# Pnl Manual

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## Contents

1	Intr	roduction	1					
	1.1	What is Pnl	1					
	1.2	A few helpful conventions	1					
	1.3	Using Pnl	4					
<b>2</b>	Obj	Objects						
	2.1		6					
	2.2	List object	8					
	2.3	· ·	9					
3	Ma	Mathematical framework 10						
	3.1	General tools	10					
	3.2		13					
4	Line	ear Algebra 1	.7					
	4.1		١7					
	4.2	Compact Vectors	25					
	4.3	*	26					
	4.4		39					
	4.5	9	13					
	4.6		16					
	4.7	v •	18					
5	Cur	mulative distribution Functions 5	3					
6	Rar	ndom Number Generators 5	5					
	6.1	The rng interface	55					
	6.2		60					
7	Function bases and regression 65							
	7.1	Overview	3					
	7.2	Functions	34					
8	Nui	merical integration 6	8					
	8.1	Overview	38					
	8.2	Functions	39					

9	Fast Fourier Transform	<b>7</b> 0
	9.1 Overview	70
	9.2 Functions	71
10	Inverse Laplace Transform	73
11	Ordinary differential equations	74
	11.1 Overview	74
	11.2 Functions	74
12	Nonlinear Constrained Optimization	<b>7</b> 5
	12.1 Overview	75
	12.2 Functions	76
13	Root finding	77
	13.1 Overview	77
	13.2 Functions	79
14	Special functions	81
	14.1 Real Bessel functions	81
	14.2 Complex Bessel functions	82
	14.3 Error functions	82
	14.4 Gamma functions	83
	14.5 Digamma function	83
	14.6 Incomplete Gamma functions	83
	14.7 Exponential integrals	84
	14.8 Hypergeometric functions	85
15	Some bindings	85
	15.1 MPI bindings	85
	15.2 The save/load interface	87
16	Financial functions	87

## 1 Introduction

## 1.1 What is Pnl

Pnl is a scientific library written in C and distributed under the Gnu Lesser General Public Licence (LGPL). This manual is divided into four parts.

- Mathematical functions: complex numbers, special functions, standard financial functions for the Black & Scholes model.
- Linear algebra : vectors, matrices, hypermatrices, tridiagonal matrices, band matrices and the corresponding routines to manipulate them and solve linear systems.
- Probabilistic functions: random number generators and cumulative distribution functions.

• Deterministic toolbox : FFT, Laplace inversion, numerical integration, zero searching, multivariate polynomial regression, ...

## 1.2 A few helpful conventions

 All header file names are prefixed by pnl\_ and are surrounded by the preprocessor conditionals

```
#ifndef _PNL_MATRIX_H
#define _PNL_MATRIX_H
...
#endif /* _PNL_MATRIX_H
```

All the header files are protected by an extern "C" declaration for possible use with a C++ compiler. The header files must be include using

```
#include "pnl/pnl_xxx.h"
```

• All function names are prefixed by pnl\_ except those implementing complex number arithmetic which are named following the C99 complex library but using a capitalised first letter C.

For example, the addition of two complex numbers is performed by the function Cadd.

- Function containing \_create in their names always return a pointer to an object created by one or several calls to dynamic allocation. Once these objects are not used, they must be freed by calling the same function but ending in \_free. A function pnl\_foo\_create\_yyy returns a PnlFoo \* object (note the "\*") and a function pnl\_foo\_bar\_create\_yyy returns a PnlFooBar \* object (note the "\*"). These objects must be freed by calling respectively pnl\_foo\_free or pnl\_foo\_bar\_free.
- Every object must implement a pnl\_xxx\_new function which returns a pointer to an empty object with all its elements properly set to 0. This means that the objects returned by the pnl\_xxx\_new functions can be used as output arguments for functions ending in \_inplace for instance. They are suitable for being resized.
- Functions containing \_wrap\_ in their names always return an object, not a pointer to an object, and do not make any use of dynamic allocation. The returned object must not be freed. For instance, a function pnl\_foo\_wrap\_xxx returns an object PnlFoo and a function pnl\_foo\_bar\_wrap\_xxx returns an object PnlFooBar

```
PnlVectComplex *v1;
PnlVectComplex v2;
v1 = pnl_vect_complex_create_from_complex (5, Complex(0., 1.));
v2 = pnl_vect_complex_wrap_subvect (v1, 1, 2);
```

```
pnl_vect_complex_free (&v1);
```

The vector v1 is of size 5 and contains the pure imaginary number i. The vector v2 only provides a view to v1(1:1+2), which means that modifying v2 will also modify v1 and vice-versa because v1 shares part of its data with v2. Note that only v1 must be freed and **not** v2.

- Functions ending in \_init do not create any object but only perform some internal initialisation.
- Hypermatrices, matrices and vectors are stored using a flat block of memory obtained by concatenating the matrix rows and C-style pointer-to-pointer arrays. Matrices are stored in row-major order, which means that the column index moves continuously. Note that this convention is not *Blas & Lapack* compliant since Fortran expects 2-dimensional arrays to be stored in a column-major order.
- Type names always begin with Pnl, they do not contain underscores but instead we use capital letters to separate units in type names.

  Examples: PnlMat, PnlMatComplex.
- Object and function names are intimately linked: an object PnlFoo is manipulated by functions starting in pnl\_foo, an object PnlFooBar is manipulated by functions starting in pnl\_foo\_bar. In table 1, we summarise the types and their corresponding prefixes.
- All macro names begin with PNL and are capitalised.
- Differences between **copy** and **clone** methods. The **copy** methods take a single argument and return a pointer to an object of the same type which is an independent copy of its argument. Example:

```
PnlVect *v1, *v2;
v1 = pnl_vect_create_from_double (5, 2.5);
v2 = pnl_vect_copy (v1);
```

v1 and v2 are two vectors of size 5 with all their elements equal to 2.5. Note that v2 must not have been created by a call to pnl\_vect\_create\_xxx because otherwise it will cause a memory leak. v1 and v2 are independent in the sense that a modification to one of them does not affect the other.

The clone methods take two arguments and fill the first one with the second one. Example:

```
PnlVect *v1, *v2;
v1 = pnl_vect_create_from_double (5, 2.5);
v2 = pnl_vect_new ();
pnl_vect_clone (v2, v1);
```

Pnl types	Pnl prefix
PnlVect	pnl_vect
PnlVectComplex	pnl_vect_complex
PnlVectInt	pnl_vect_int
PnlMat PnlMatComplex PnlMatInt	pnl_mat pnl_mat_complex pnl_mat_int
PnlHmat	pnl_hmat
PnlHmatComplex	pnl_hmat_complex
PnlHmatInt	pnl hmat int
PnlTridiagMat PnlBandMat	pnl_tridiag_mat pnl_band_mat
PnlList	pnl_list
PnlBasis	pnl_basis
PnlCgSolver	pnl_cg_solver
PnlBicgSolver	pnl_bicg_solver
${\bf PnlGmresSolver}$	pnl_gmres_solver

Figure 1: Pnl types

v1 and v2 are two vectors of size 5 with all their elements equal to 2.5. Note that v2 must have been created by a call to pnl\_vect\_new because otherwise the function pnl\_vect\_clone will crash. v1 and v2 are independent in the sense that a modification to one of them does not modify the other.

- All objects are measured using integers int and not size\_t. Hence, iterations over vectors, matrices, ... should use an index of type int.
- In fonctions ending in **inplace**, the output parameter must be different from any of the input parameters.

## 1.3 Using Pnl

In this section, we assume that the library is installed in the directory \$HOME/pnl-xxx. Once the library has been installed, the libraries can be found in the \$HOME/pnl-xxx/lib directory and the headers in the \$HOME/pnl-xxx/include directory.

## 1.3.1 Compiling and Linking

The header files of the library are installed in a root pnl directory and should always be included with this pnl/ prefix. So, for instance to use random number generators you should include

```
#include <pnl/pnl_random.h>
```

Compiling and linking by hand If gcc is used, you should pass the following options

- -I\$HOME/pnl-xxx/include for compiling
- -L\$HOME/pnl-xxx/lib -lpnl for linking

This does not work straight away on all OS especially if the library is not installed in a standard directory namely /usr/ or /usr/local/ for which you need a privileged writing access. On some systems, you may need to add to the linker flags the dependencies of the library, which can become very tedious. Therefore, we provide a second automatic mechanism which takes care of the dependencies on its own.

Compiling and linking using an automatic Makefile This mechanism only works under Unix (it has been tested under various Linux distributions and Mac OS X).

First, you need to create a new directory wherever you want, put in all your code and create a Makefile as below

To define your target just add the executable name, say my-exec, to the BINS list and create an entry my\_exec\_SRC carrying the list of source files needed to create your executable. Note that if dashes '-' may appear in an executable name, the name of the associated variable holding the list of source files is obtained by replacing dashes with underscores '\_' and adding the SRC suffix.

Assume you want to create two binaries: my-exec based on mixed C and C++ code (file1.c and file2.cpp) and mybinary based on pool.cxx and pool.cxp. You can use the following Makefile.

```
## Flags passed to the linker
LDFLAGS=
## Flags passed to the compiler
CFI.AGS=
## list of executables to create
BINS=my-exec mybinary
my_exec_SRC=file1.c file2.cpp
# optional flags for compiling and linking
my_exec_CFLAGS=
my exec CXXFLAGS=
my_exec_LDFLAGS=
mybinary_SRC=poo1.cxx poo2.cpp
# optional flags for compiling and linking
mybinary_CFLAGS=
mybinary_CXXFLAGS=
mybinary_LDFLAGS=
```

```
## This line must be the last one
include full_path_to_pnl_build/CMakeuser.incl
```

Let us comment a little the different variables

- CFLAGS: global flags used for creating objects based on C code
- CXXFLAGS: global flags used for creating objects based on C++ code
- LDFLAGS: gobal linker flags.
- binaryname\_CFLAGS: flags used when creating the objects based on C code and required by binaryname
- binaryname\_CXXFLAGS: flags used when creating the objects based on C++ code and required by binaryname
- binaryname\_LDFLAGS: flags used when linking objects for creating binaryname

An example of such a Makefile can be found in pnl-xxx/perso.

Warning: if a file appears in the source list of several binairies, the flags used to compile this file are determined by the ones of the first binary involving this file. In the following example main.cpp will always be compiled with the flag -03 even for generating bin2

```
BINS=bin1 bin2
```

```
bin1_SRC=main.cpp poo1.c
my_exec_CXXFLAGS=-03
bin2_SRC=main.cpp poo2.c
mybinary_CXXFLAGS=-g -00
## This line must be the last one
include full_path_to_pnl_build/CMakeuser.incl
```

## 2 Objects

## 2.1 The top-level object

The PnlObject structure is used to simulate some inheritance between the ojbects of Pnl. It must be the first element of all the objects existing in Pnl so that casting any object to a PnlObject is legal

```
typedef unsigned int PnlType;

typedef void (DestroyFunc) (void **);
typedef PnlObject* (CopyFunc) (PnlObject *);
typedef PnlObject* (NewFunc) (PnlObject *);
typedef void (CloneFunc) (PnlObject *dest, const PnlObject *src);
```

Description
general vectors
real vectors
integer vectors
complex vectors
general matrices
real matrices
integer matrices
complex matrices
general tridiagonal matrices
real tridiagonal matrices
general band matrices
real band matrices
general hyper matrices
real hyper matrices
integer hyper matrices
complex hyper matrices
bases
random number generators
doubly linked list

Table 1: PnlTypes

Here is the list of all the types actually defined We provide several macros for manipulating PnlObejcts.

- PNL\_OBJECT (o)

  Description Cast any object into a PnlObject
- PNL\_VECT\_OBJECT (o)
  Description Cast any object into a PnlVectObject
- PNL\_MAT\_OBJECT (o)

  Description Cast any object into a PnlMatObject
- PNL\_HMAT\_OBJECT (o)
  Description Cast any object into a PnlHmatObject

- PNL\_BAND\_MAT\_OBJECT (o)
  Description Cast any object into a PnlBandMatObject
- PNL\_TRIDIAGMAT\_OBJECT (o)
  Description Cast any object into a PnlTridiagMatObject
- PNL\_BASIS\_OBJECT (o)

  Description Cast any object into a PnlBasis
- PNL\_RNG\_OBJECT (o)
  Description Cast any object into a PnlRng
- PNL\_LIST\_OBJECT (o)

  Description Cast any object into a PnlList
- PNL\_GET\_TYPENAME (o)

  Description Return the name of the type of any object inheriting from PnlObject
- PNL\_GET\_TYPE (o)

  Description Return the type of any object inheriting from PnlObject
- PNL\_GET\_PARENT\_TYPE (o)

  Description Return the parent type of any object inheriting from PnlObject
- PnlObject\* pnl\_object\_create (PnlType t)
  Description Create an empty PnlObject of type t which can any of the registered types, see Table 1.

## 2.2 List object

This section describes functions for creating an manipulating lists. Lists are internally stored as doubly linked lists.

The structures and functions related to lists are declared in pnl/pnl\_list.h.

```
typedef struct _PnlCell PnlCell;
struct _PnlCell
{
   struct _PnlCell *prev; /*!< previous cell or 0 */
   struct _PnlCell *next; /*!< next cell or 0 */
   PnlObject *self; /*!< stored object */
};

typedef struct _PnlList PnlList;
struct _PnlList
{
   /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlList pointer to be cast to a PnlObject
   */</pre>
```

- PnlList \* pnl\_list\_new ()
  Description Create an empty list
- PnlCell \* pnl\_cell\_new ()
  Description Create an cell list
- PnlList\* pnl\_list\_copy (const PnlList\*A)

  Description Create a copy of a PnlList. Each element of the list A is copied by calling the its copy member.
- void pnl\_list\_clone (PnlList \*dest, const PnlList\*src)

  Description Copy the content of src into the already existing list dest. The list dest is automatically resized. This is a hard copy, the contents of both lists are independent after cloning.
- void **pnl\_list\_free** (**PnlList** \*\*L)

  Description Free a list
- void **pnl\_cell\_free** (PnlCell \*\*c)
  Description Free a list
- PnlObject\* pnl\_list\_get ( PnlList \*L, int i)

  Description This function returns the content of the i-th cell of the list L. This function is optimized for linearly accessing all the elements, so it can be used inside a for loop for instance.
- void pnl\_list\_insert\_first (PnlList \*L, PnlObject \*o)

  Description Insert the object o on top of the list L. Note that o is not copied in L, so do not free o yourself, it will be done automatically when calling pnl list free
- void pnl\_list\_insert\_last (PnlList \*L, PnlObject \*o)
   Description Insert the object o at the bottom of the list L. Note that o is not copied in L, so do not free o yourself, it will be done automatically when calling pnl\_list\_free
- void pnl\_list\_remove\_last (PnlList \*L)
   Description Remove the last element of the list L and frees it.
- void pnl\_list\_remove\_first (PnlList \*L)
   Description Remove the first element of the list L and frees it.

- void **pnl\_list\_remove\_i** (**PnlList** \*L, int i)

  Description Remove the i-th element of the list L and frees it.
- void pnl\_list\_concat (PnlList \*L1, PnlList \*L2)
   Description Concatenate the two lists L1 and L2. The resulting list is store in L1 on exit.
   Do not free L2 since concatenation does not actually copy objects but only manipulates addresses.
- void pnl\_list\_print (const PnlList \*L)

  Description Only prints the types of each element. When the PnlObject object has a print member, we will use it.

## 2.3 Array object

This section describes functions for creating and manipulating arrays of PnlObjects. The structures and functions related to arrays are declared in pnl/pnl\_array.h.

```
typedef struct _PnlArray PnlArray;
struct _PnlArray
{
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlArray pointer to be cast to a PnlObject
    */
    PnlObject object;
    int size;
    PnlObject **array;
    int mem_size;
};
```

- PnlArray \* pnl\_array\_new ()
  Description Create an empty array
- PnlArray \* pnl\_array\_create (int n)
  Description Create an array of length n.
- PnlArray\* pnl\_array\_copy (const PnlArray\*A)

  Description Create a copy of a PnlArray. Each element of the array A is copied by calling the A[i].object.copy.
- void pnl\_array\_clone (PnlArray \*dest, const PnlArray\*src)

  Description Copy the content of src into the already existing array dest. The array dest is automatically resized. This is a hard copy, the contents of both arrays are independent after cloning.
- void **pnl\_array\_free** (PnlArray \*\*)

  Description Free an array and all the objects hold by the array.
- int pnl\_array\_resize (PnlArray \*T, int size)

  Description Resize T to be size long. As much as possible of the original data is kept.

- PnlObject\* pnl\_array\_get ( PnlArray \*T, int i)

  Description This function returns the content of the i-th cell of the array T. No copy is made.
- PnlObject\* pnl\_array\_set ( PnlArray \*T, int i, PnlObject\*O)

  Description T[i] = 0. No copy is made, so the object 0 must not be freed manually.
- void pnl\_array\_print (PnlArray \*)

  Description Not yet implemented because it would require that the structure PnlObject has a field copy.

## 3 Mathematical framework

#### 3.1 General tools

The macros and functions of this paragraph are defined in pnl/pnl mathtools.h.

#### 3.1.1 Constants

A few mathematical constants are provided by the library. Most of them are actually already defined in math.h, values.h or limits.h and a few others have been added.

```
\mathbf{M}_{\mathbf{L}}\mathbf{E}
M_LOG2E
                             \log_2 e
M_LOG10E
                             \log_{10} e
M LN2
                             \log_e 2
M_LN10
                             \log_e 10
M PI
                             \pi
M 2PI
                             2\pi
M PI 2
                             \pi/2
M PI 4
                             \pi/4
M_1PI
                             1/\pi
M 2 PI
                             2/\pi
M 2 SQRTPI
                             2/\sqrt{\pi}
                             sqrt2\pi
M_SQRT2PI
                              \sqrt{2}
M_SQRT2
                             \gamma = \lim_{n \to \infty} \left( \sum_{k=1}^{n} \frac{1}{k} - \ln(n) \right)
M EULER
                              1/\sqrt{2}
M_SQRT1_2
                              1/\sqrt{2\pi}
M 1 SQRT2PI
M SQRT2 PI
                              \sqrt{2/\pi}
INT MAX
                             2147483647
MAX_INT
                             INT_MAX
DBL MAX
                             1.79769313486231470e + 308
DOUBLE MAX
                             DBL MAX
DBL EPSILON
                             2.2204460492503131e - 16
PNL_NEGINF
                              -\infty
PNL_POSINF
                             +\infty
PNL_INF
                              +\infty
                             Not a Number
NAN
```

#### 3.1.2 A few macros

- PNL\_IS\_ODD (int n)
  Description Return 1 if n is odd and 0 otherwise.
- PNL\_IS\_EVEN (int n)
  Description Return 1 if n is even and 0 otherwise.
- PNL\_ALTERNATE (int n)
  Description Return (-1)<sup>n</sup>.
- MIN (x,y)

  Description Return the minimum of x and y.
- MAX (x,y)

  Description Return the maximum of x and y.
- ABS (x)

  Description Return the absolute value of x.
- PNL\_SIGN (x)

  Description Return the sign of x (-1 if x < 0, 0 otherwise).
- SQR (x) Description Return  $x^2$ .
- CUB (x) Description Return  $x^3$ .

## 3.1.3 Functions

We provide a few functions mathematical functions named pnl\_funcname, some of them may be available in C99 as funcname.

- int pnl\_itrunc (double s)

  Description This function is similar to the trunc function (provided by the C library)
  but the result is typed as an integer instead of a double. Digits may be lost if s exceeds
  MAX\_INT.
- long int **pnl\_ltrunc** (double s)

  Description This function is similar to the **trunc** function (provided by the C library) but the result is typed as a long integer instead of a double.
- double **pnl\_trunc** (double s)

  Description Return the nearest integer not greater than the absolute value of s. This function is part of C99 as trunc.
- double pnl\_round (double s)

  Description Return the integral value nearest to x rounding half-way cases away from zero, regardless of the current rounding direction. This function is part of C99 as round.

- int pnl\_iround (double s)

  Description This function is similar to the round function (provided by the C library)
  but the result is typed as an integer instead of a double. Digits may be lost if s exceeds
  MAX\_INT.
- long int **pnl\_lround** (double s)

  Description This function is similar to the **round** function (provided by the C library) but the result is typed as a long integer instead of a double.
- double pnl\_lgamma (double x) Description Compute  $\log(\Gamma(x))$ .
- double **pnl\_tgamma** (double x) Description Compute  $\Gamma(x)$ .
- double pnl\_acosh (double x)
   Description Compute acosh(x).
- double pnl\_asinh (double x)
   Description Compute asinh(x).
- double pnl\_atanh (double x)
   Description Compute atanh(x).
- double pnl\_log1p (double x)
   Description Compute log(1+x) accurately for small values of x
- double pnl\_expm1 (double x)
   Description Compute exp(x)-1 accurately for small values of x
- double pnl\_cosm1 (double x)
   Description Compute cos(x)-1 accurately for small values of x

## 3.2 Complex numbers

### 3.2.1 Overview

The complex type and related functions are defined in the header pnl/pnl\_complex.h.

The first native implementation of complex numbers in the C language appeared in C99, which is unfortunately not available on all platforms. For this reason, we provide here an implementation of complex numbers.

```
typedef struct {
   double r; /*!< real part */
   double i; /*!< imaginary part */
} dcomplex;</pre>
```

#### 3.2.2 Constants

CZERO 0 as a complex number
CONE 1 as a complex number
CI I the unit complex number

#### 3.2.3 Functions

- double Creal (dcomplex z) Description R(z)
- double Cimag (dcomplex z) Description Im(z)
- dcomplex Cadd (dcomplex z, dcomplex b)
   Description z+b
- dcomplex **CRadd** (dcomplex z, double b)

  Description z+b
- dcomplex RCadd (double b, dcomplex z)
   Description b+z
- dcomplex Csub (dcomplex z, dcomplex b)

  Description z-b
- dcomplex CRsub (dcomplex z, double b)
   Description z-b
- dcomplex RCsub (double b, dcomplex z)
   Description b-z
- dcomplex Cminus (dcomplex z)
   Description -z
- dcomplex Cmul (dcomplex z, dcomplex b)

  Description z\*b
- dcomplex **RCmul** (double x, dcomplex z) Description x\*z
- dcomplex CRmul (dcomplex z, double x)
   Description z \* x
- dcomplex CRdiv (dcomplex z, double x)
   Description z/x
- dcomplex RCdiv (double x, dcomplex z)
   Description x/z
- dcomplex Complex (double x, double y)
   Description x + i y
- dcomplex\_polar (double r, double theta)

  Description r exp(i theta)
- dcomplex Conj (dcomplex z) Description  $\overline{z}$

- dcomplex Cinv (dcomplex z)
  Description 1/z
- dcomplex Cdiv (dcomplex z, dcomplex w)

  Description z/w
- double Csqr\_norm (dcomplex z) Description  $Re(z)^2 + im(z)^2$
- double Cabs (dcomplex z)

  Description |z|
- dcomplex Csqrt (dcomplex z)

  Description sqrt(z), square root (with positive real part)
- dcomplex Clog (dcomplex z)
  Description log(z)
- dcomplex Cexp (dcomplex z)

  Description exp(z)
- dcomplex CIexp (double t)

  Description exp( it )
- dcomplex Cpow (dcomplex z, dcomplex w) Description  $z^w$ , power function
- dcomplex Cpow\_real (dcomplex z, double x) Description  $z^x$ , power function
- dcomplex Ccos (dcomplex z)

  Description cos(g)
- dcomplex Csin (dcomplex z)

  Description sin(g)
- dcomplex Ctan (dcomplex z)

  Description tan(z)
- dcomplex Ccotan (dcomplex z)

  Description cotan(z)
- dcomplex Ccosh (dcomplex z)
  Description cosh(g)
- dcomplex Csinh (dcomplex z)
  Description sinh(g)
- dcomplex Ctanh (dcomplex z) Description  $tanh(z) = \frac{1-e^{-2z}}{1+e^{-2z}}$
- dcomplex Ccotanh (dcomplex z) Description cotanh(z) =  $\frac{1+e^{-2z}}{1-e^{-2z}}$

- double Carg (dcomplex z)

  Description arg(z)
- dcomplex Ctgamma (dcomplex z)

  Description Gamma(z), the Gamma function
- dcomplex Clgamma (dcomplex z)

  Description log(Gamma (z)), the logarithm of the Gamma function
- void **Cprintf** (dcomplex z)

  Description Print a complex number on the standard output

Most algebraic operations on complex numbers are implemented using the following naming for the functions

- All these function names begin in C\_op\_,
- The small letters a, b denote two complex numbers whereas d is a real number,
- The letter i denotes the multiplication by the pure imagniary number i,
- The letter c indicates that the next coming number is conjugated.
- The letters p, m denote the two standard operations plus and minus respectively.

For example C\_op\_idamcb is  $id(a-\overline{b})$ . So functions are :

- dcomplex C\_op\_apib (dcomplex a, dcomplex b) Description a + ib.
- dcomplex C\_op\_apcb (dcomplex a, dcomplex b) Description  $a + \overline{b}$ .
- dcomplex C\_op\_amcb (dcomplex a, dcomplex b) Description  $a \bar{b}$ .
- dcomplex C\_op\_amib (dcomplex a, dcomplex b)
   Description a i b
- dcomplex  $C_{op}_{dapb}$  (double d, dcomplex a, dcomplex b) Description d(a + b).
- dcomplex C\_op\_damb (double d, dcomplex a, dcomplex b) Description d(a-b).
- dcomplex C\_op\_dapib (double d, dcomplex a, dcomplex b) Description d(a + ib).
- dcomplex C\_op\_damib (double d, dcomplex a, dcomplex b) Description d(a ib).
- dcomplex **C\_op\_dapcb** (double d, dcomplex a, dcomplex b) Description  $d\left(a+\overline{b}\right)$ .

- dcomplex **C\_op\_damcb** (double d, dcomplex a, dcomplex b) Description  $d\left(a-\bar{b}\right)$ .
- dcomplex  $C_{op_idapb}$  (double d, dcomplex a, dcomplex b) Description id(a + b).
- dcomplex **C\_op\_idamb** (double d, dcomplex a, dcomplex b) Description id(a b).
- dcomplex C\_op\_idapcb (double d, dcomplex a, dcomplex b) Description  $id\left(a+\bar{b}\right)$ .
- dcomplex **C\_op\_idamcb** (double d, dcomplex a, dcomplex b) Description  $id(a \bar{b})$ .

## 4 Linear Algebra

#### 4.1 Vectors

#### 4.1.1 Overview

The structures and functions related to vectors are declared in pnl/pnl\_vector.h. Vectors are declared for several basic types: double, int, and dcomplex. In the following declarations, BASE must be replaced by one the previous types and the corresponding vector structures are respectively named PnlVect, PnlVectInt, PnlVectComplex

```
typedef struct _PnlVect {
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlVect pointer to be cast to a PnlObject
 PnlObject object;
 int size; /*!< size of the vector */
 int mem_size; /*!< size of the memory block allocated for array */
 double *array; /*!< pointer to store the data */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlVect;
typedef struct _PnlVectInt {
 /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlVectInt pointer to be cast to a PnlObject
   */
 PnlObject object;
 int size; /*!< size of the vector */
 int mem_size; /*!< size of the memory block allocated for array */
 int *array; /*!< pointer to store the data */
 int owner; /*!< 1 if the object owns its array member, 0 otherwise */
```

```
} PnlVectInt;

typedef struct _PnlVectComplex {
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlVectComplex pointer to be cast
    * to a PnlObject
    */
    PnlObject object;
    int size; /*!< size of the vector */
    int mem_size; /*!< size of the memory block allocated for array */
    dcomplex *array; /*!< pointer to store the data */
    int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlVectComplex;</pre>
```

size is the size of the vector, array is a pointer containing the data and owner is an integer to know if the vector owns its array pointer (owner=1) or shares it with another structure (owner=0). mem\_size is the number of elements the vector can hold at most.

#### 4.1.2 Functions

General functions These functions exist for all types of vector no matter what the basic type is. The following conventions are used to name functions operating on vectors. Here is the table of prefixes used for the different basic types.

type	prefix	BASE
double	pnl_vect	double
int	pnl_vect_int	int
dcomplex	pnl_vect_complex	dcomplex

In this paragraph, we present the functions operating on PnlVect which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_vect and double according the above table.

Constructors and destructors There are no special functions to access the size of a vector, instead the field size should be accessed directly.

- PnlVect \* pnl\_vect\_new ()
  Description Create a new PnlVect of size 0.
- PnlVect \* pnl\_vect\_create (int size)
  Description Create a new PnlVect pointer.
- PnlVect \* pnl\_vect\_create\_from\_zero (int size)
  Description Create a new PnlVect pointer and sets it to zero.
- PnlVect \* pnl\_vect\_create\_from\_double (int size, double x)
  Description Create a new PnlVect pointer and sets all elements t x.

- PnlVect \* pnl\_vect\_create\_from\_ptr (int size, const double \*x)

  Description Create a new PnlVect pointer and copies x to array.
- PnlVect \* pnl\_vect\_create\_from\_list (int size, ...)

  Description Create a new PnlVect pointer of length size filled with the extra arguments passed to the function. The number of extra arguments passed must be equal to size and they must be of the type BASE. Example: To create a vector {1., 2.}, you should enter pnl\_vect\_create\_from\_list(2, 1.0, 2.0) and NOT pnl\_vect\_create\_from\_list(2, 1.0, 2) or pnl\_vect\_create\_from\_list(2, 1, 2.0). Be aware that this cannot be checked inside the function.
- PnlVect \* pnl\_vect\_create\_from\_file (const char \*file)

  Description Read a vector from a file and creates the corresponding PnlVect. The data might be stored as a single blank separated line or as a one column file with one element per line.
- PnlVect \* pnl\_vect\_copy (const PnlVect \*v)

  Description This is a copying constructor. It creates a copy of a PnlVect.
- void pnl\_vect\_clone (PnlVect \*clone, const PnlVect \*v)

  Description Clone a PnlVect. clone must be an already existing PnlVect. It is resized to match the size of v and the data are copied. Future modifications to v will not affect clone.
- PnlVect \* pnl\_vect\_create\_subvect\_with\_ind (const PnlVect \*V, const PnlVectInt \*ind)

  Description Create a new vector containing V(ind(:)).
- void pnl\_vect\_extract\_subvect\_with\_ind (PnlVect \*V\_sub, const PnlVect \*V, const PnlVectInt \*ind)

  Description On exit, V\_sub = V(ind(:)).
- PnlVect \* pnl\_vect\_create\_subvect (const PnlVect \*V, int i, int len)
  Description Create a new vector containing V(i:i+len-1). The elements are copied.
- void pnl\_vect\_extract\_subvect (PnlVect \*V\_sub, const PnlVect \*V, int i, int len)

  Description On exit, V\_sub = V(i:i+len-1). The elements are copied.
- void **pnl\_vect\_free** (PnlVect \*\*v)

  Description Free a PnlVect pointer and set the data pointer to NULL
- PnlVect pnl\_vect\_wrap\_array (const double \*x, int size)

  Description Create a PnlVect containing the data x. No copy is made. It is just a container.
- PnlVect pnl\_vect\_wrap\_subvect (const PnlVect \*x, int i, int s)

  Description Create a PnlVect containing x(i:i+s-1). No copy is made. It is just a container. The returned PnlVect has size=s and owner=0.
- PnlVect pnl\_vect\_wrap\_subvect\_with\_last (const PnlVect \*x, int i, int j)

  Description Create a PnlVect containing x(i:j). No copy is made. It is just a container.

• PnlVect pnl\_vect\_wrap\_mat (const PnlMat \*M)

Description Return a PnlVect (not a pointer) whose array is the row wise array of M.

The new vector shares its data with the matrix M, which means that any modification to one of them will affect the other.

## Resizing vectors

- int pnl\_vect\_resize (PnlVect \*v, int size)

  Description Resize a PnlVect. It copies as much of the old data to fit in the resized object.
- int pnl\_vect\_resize\_from\_ptr (PnlVect \*v, int size, double \*t)

  Description Resize a PnlVect and uses t to fill the vector. t must be of size size.

- void **pnl\_vect\_set** (**PnlVect** \*v, int i, double x)

  Description Set v[i]=x
- double **pnl\_vect\_get** (const **PnlVect** \*v, int i) Description Return the value of v[i].
- void **pnl\_vect\_lget** (**PnlVect** \*v, int i) Description Return the address of v[i].
- void **pnl\_vect\_set\_double** (**PnlVect** \*v, double x) Description Set all elements to x.
- void pnl\_vect\_set\_zero (PnlVect \*v)
  Description Set all elements to zero.

Equivalently to these functions, there exist macros for **PnlVect only**.

- GET (v, i)

  Description Return v[i] for reading, eg. x=LET(v,i)
- LET (v, i)

  Description Return v[i] as a lvalue for writing, eg. LET(v,i)=x

#### Printing vector

- void pnl\_vect\_print (const PnlVect \*V)
   Description Print a PnlVect as a column vector
- void **pnl\_vect\_fprint** (FILE \*fic, const **PnlVect** \*V)

  Description Print a **PnlVect** in file **fic** as a column vector.
- void pnl\_vect\_print\_asrow (const PnlVect \*V)

  Description Print a PnlVect as a row vector

- void pnl\_vect\_fprint\_asrow (FILE \*fic, const PnlVect \*V)

  Description Print a PnlVect in file fic as a row vector.
- void pnl\_vect\_print\_nsp (const PnlVect \*V)

  Description Print a vector to the standard output in a format compatible with Nsp.
- void **pnl\_vect\_fprint\_nsp** (FILE \*fic, const **PnlVect** \*V)

  Description Print a vector to a file in a format compatible with Nsp.

## Applying external operation to vectors

- void pnl\_vect\_minus (PnlVect \*lhs)

  Description In-place unary minus
- void **pnl\_vect\_plus\_double** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar addition
- void **pnl\_vect\_minus\_double** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar substraction
- void **pnl\_vect\_mult\_double** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar multiplication
- void **pnl\_vect\_div\_double** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar division

## Element wise operations

- void pnl\_vect\_plus\_vect (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector addition
- void pnl\_vect\_minus\_vect (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector substraction
- void pnl\_vect\_inv\_term (PnlVect \*lhs)
   Description In-place term by term vector inversion
- void pnl\_vect\_div\_vect\_term (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place term by term vector division
- void pnl\_vect\_mult\_vect\_term (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector term by term multiplication
- void pnl\_vect\_map (PnlVect \*lhs, const PnlVect \*rhs, double(\*f)(double))
   Description lhs = f(rhs)
- void pnl\_vect\_map\_inplace (PnlVect \*lhs, double(\*f)(double))
   Description lhs = f(lhs)
- void pnl\_vect\_map\_vect (PnlVect \*lhs, const PnlVect \*rhs1, const PnlVect \*rhs2, double(\*f)(double, double))
   Description 1hs = f(rhs1, rhs2)

- void pnl\_vect\_map\_vect\_inplace (PnlVect \*lhs, PnlVect \*rhs, double(\*f)(double,double))

  Description lhs = f(lhs,rhs)
- void **pnl\_vect\_axpby** (double a, const **PnlVect** \*x, double b, **PnlVect** \*y)

  Description Compute y: = a x + b y. When b==0, the content of y is not used on input and instead y is resized to match x.
- double pnl\_vect\_sum (const PnlVect \*lhs)
   Description Return the sum of all the elements of a vector
- void pnl\_vect\_cumsum (PnlVect \*lhs)

  Description Compute the cumulative sum of all the elements of a vector. The original vector is modified
- double pnl\_vect\_prod (const PnlVect \*V)
   Description Return the product of all the elements of a vector
- void pnl\_vect\_cumprod (PnlVect \*lhs)

  Description Compute the cumulative product of all the elements of a vector. The original vector is modified

## Scalar products and norms

- double pnl\_vect\_norm\_two (const PnlVect \*V)

  Description Return the two norm of a vector
- double pnl\_vect\_norm\_one (const PnlVect \*V)

  Description Return the one norm of a vector
- double **pnl\_vect\_norm\_infty** (const **PnlVect** \*V)

  Description Return the infinity norm of a vector
- double pnl\_vect\_scalar\_prod (const PnlVect \*rhs1, const PnlVect \*rhs2)

  Description Compute the scalar product between 2 vectors
- int pnl\_vect\_cross (PnlVect \*lhs, const PnlVect \*x, const PnlVect \*y)

  Description Compute the cross product of x and y and store the result in lhs. The vectors x and y must be of size 3 and FAIL is returned otherwise.
- double pnl\_vect\_dist (const PnlVect \*x, const PnlVect \*y) Description Compute the distance between x and y, ie  $\sqrt{\sum_i |x_i y_i|^2}$ .

## Test functions

- int pnl\_vect\_eq (const PnlVect \*V1, const PnlVect \*V2)

  Description Test if two vectors are equal. Returns TRUE or FALSE.
- int pnl\_vect\_eq\_double (const PnlVect \*v, double x)

  Description Test if all the components of v are equal to x. Returns TRUE or FALSE.

**Ordering functions** The following functions are not defined for PnlVectComplex because there is no total ordering on Complex numbers

- double pnl\_vect\_max (const PnlVect \*V)
   Description Return the maximum of a a vector
- double **pnl\_vect\_min** (const **PnlVect** \*V)

  Description Return the minimum of a vector
- void pnl\_vect\_minmax (double \*m, double \*M, const PnlVect \*)

  Description Compute the minimum and maximum of a vector which are returned in m and M respectively.
- void pnl\_vect\_min\_index (double \*m, int \*im, const PnlVect \*)
   Description Compute the minimum of a vector and its index stored in sets m and im respectively.
- void pnl\_vect\_max\_index (double \*M, int \*iM, const PnlVect \*)
   Description Compute the maximum of a vector and its index stored in sets m and im respectively.
- void pnl\_vect\_minmax\_index (double \*m, double \*M, int \*im, int \*iM, const PnlVect \*)

  Description Compute the minimum and maximum of a vector and the corresponding indices stored respectively in m, M, im and iM.
- void pnl\_vect\_qsort (PnlVect \*, char order)
   Description Sort a vector using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing).
- void pnl\_vect\_qsort\_index (PnlVect \*, PnlVectInt \*index, char order)

  Description Sort a vector using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing). On output, index contains the permutation used to sort the vector.
- int pnl\_vect\_find (PnlVectInt \*ind, char \*type, int(\*f)(double \*t), ...)

  Description f is a function taking a C array as argument and returning an integer. type is a string composed by the letters 'r' and 'v' and is used to describe the types of the arguments appearing after f. This function aims at simulating Scilab's find function. Here are a few examples (capital letters are used for vectors and small letters for real values)

```
- ind = find ( a < X )
        int isless ( double *t ) { return t[0] < t[1]; }
        pnl_vect_find ( ind, "rv", isless, a, X );

- ind = find (X <= Y)
        int isless ( double *t ) { return t[0] <= t[1]; }
        pnl_vect_find ( ind, "vv", isless, X, Y );</pre>
```

```
- ind = find ((a < X) && (X <= Y))
    int cmp ( double *t )
    {
       return (t[0] <= t[1]) && (t[1] <= t[2]);
    }
    pnl_vect_find ( ind, "rvv", cmp, a, X, Y );</pre>
```

ind contains on exit the indices i for which the function f returned 1. This function returns OK or FAIL when something went wrong (size mismatch between matrices, invalid string type).

#### Misc

- void pnl\_vect\_swap\_elements (PnlVect \*v, int i, int j)
  Description Exchange v[i] and v[j].
- void pnl\_vect\_reverse (PnlVect \*v)

  Description Perform a mirror operation on v. On output v[i] = v[n-1-i] for i=0,...,n-1 where n is the length of the vector.

## Complex vector functions

- void **pnl\_vect\_complex\_mult\_double** (**PnlVectComplex** \*lhs, double x) Description In-place multiplication by a double.
- PnlVectComplex\* pnl\_vect\_complex\_create\_from\_array (int size, const double \*re, const double \*im)

  Description Create a PnlVectComplex given the arrays of the real parts re and imaginary parts im.
- void pnl\_vect\_complex\_split\_in\_array (const PnlVectComplex \*v, double \*re, double \*im)

  Description Split a complex vector into two C arrays: the real parts of the elements of v are stored into re and the imaginary parts into im.
- void pnl\_vect\_complex\_split\_in\_vect (const PnlVectComplex \*v, PnlVect \*re, PnlVect \*im)

  Description Split a complex vector into two PnlVects: the real parts of the elements of v are stored into re and the imaginary parts into im.

There exist functions to directly access the real or imaginary parts of an element of a complex vector. These functions also have inlined versions that are used if the variable <code>HAVE\_INLINE</code> was declared at compilation time.

- double **pnl\_vect\_complex\_get\_real** (const **PnlVectComplex** \*v, int i) Description Return the real part of v[i].
- double **pnl\_vect\_complex\_get\_imag** (const **PnlVectComplex** \*v, int i) Description Return the imaginary part of v[i].

- double\* pnl\_vect\_complex\_lget\_real (const PnlVectComplex \*v, int i)

  Description Return the real part of v[i] as a lvalue.
- double\* pnl\_vect\_complex\_lget\_imag (const PnlVectComplex \*v, int i)

  Description Return the imaginary part of v[i] as a lvalue.
- void pnl\_vect\_complex\_set\_real (const PnlVectComplex \*v, int i, double re)

  Description Set the real part of v[i] to re.
- void pnl\_vect\_complex\_set\_imag (const PnlVectComplex \*v, int i, double im)

  Description Set the imaginary part of v[i] to im.

Equivalently to these functions, there exist macros. When the compiler is able to handle inline code, there is no gain in using macros instead of inlined functions at least in principle.

- GET\_REAL (v, i)

  Description Return the real part of v[i].
- **GET\_IMAG** (v, i)

  Description Return the imaginary part of v[i].
- LET\_REAL (v, i)

  Description Return the real part of v[i] as a lvalue.
- LET\_IMAG (v, i)

  Description Return the imaginary part of v[i] as a lvalue.

## 4.2 Compact Vectors

## 4.2.1 Short description

```
typedef struct PnlVectCompact {
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlVectCompact pointer to be cast to a PnlObject
    */
PnlObject object;
int size; /* size of the vector */
union {
    double val; /* single value */
    double *array; /* Pointer to double values */
};
char convert; /* 'a', 'd' : array, double */
} PnlVectCompact;
```

#### 4.2.2 Functions

• PnlVectCompact \* pnl\_vect\_compact\_new ()
Description Create a PnlVectCompact of size 0.

- PnlVectCompact \* pnl\_vect\_compact\_create (int n, double x)
  Description Create a PnlVectCompact.
- int pnl\_vect\_compact\_resize (PnlVectCompact \*v, int size, double x) Description Resize a PnlVectCompact.
- PnlVectCompact \* pnl\_vect\_compact\_copy (const PnlVectCompact\*v)

  Description Copy a PnlVectCompact
- void pnl\_vect\_compact\_free (PnlVectCompact \*\*v)
  Description Free a PnlVectCompact
- PnlVect \* pnl\_vect\_compact\_to\_pnl\_vect (const PnlVectCompact \*C)

  Description Convert a PnlVectCompact pointer to a PnlVect pointer.
- double **pnl\_vect\_compact\_get** (const **PnlVectCompact** \*C, int i) Description Access function
- void **pnl\_vect\_compact\_set\_double** (**PnlVectCompact** \*C, double x) Description Set all elements of C to x. C is converted to a compact storage.
- void pnl\_vect\_compact\_set\_ptr (PnlVectCompact \*C, double \*ptr)

  Description Copy the array ptr into C. We assume that the sizes match. C is converted to a non compact storage.

#### 4.3 Matrices

#### 4.3.1 Overview

The structures and functions related to matrices are declared in pnl/pnl\_matrix.h.

```
typedef struct _PnlMat{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlMat pointer to be cast to a PnlObject
  PnlObject object;
  int m; /*! < nb rows */
  int n; /*!< nb columns */
  int mn; /*!< product m*n */</pre>
  int mem_size; /*!< size of the memory block allocated for array */
  double *array; /*!< pointer to store the data row-wise */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMat;
typedef struct _PnlMatInt{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlMatInt pointer to be cast to a PnlObject
   */
```

```
PnlObject object;
 int m; /*!< nb rows */
 int n; /*!< nb columns */
 int mn; /*!< product m*n */
 int mem size; /*!< size of the memory block allocated for array */
 int *array; /*!< pointer to store the data row-wise */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMatInt;
typedef struct _PnlMatComplex{
 /**
  * Must be the first element in order for the object mechanism to work
  * properly. This allows any PnlMatComplex pointer to be cast
  * to a PnlObject
  */
 PnlObject object;
 int m; /*! < nb rows */
 int n; /*!< nb columns */
 int mn; /*!< product m*n */
 int mem_size; /*!< size of the memory block allocated for array */
 dcomplex *array; /*!< pointer to store the data row-wise */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMatComplex;
```

m is the number of rows, n is the number of columns. array is a pointer containing the data of the matrix stored line wise, The element (i, j) of the matrix is array[i\*m+j]. owner is an integer to know if the matrix owns its array pointer (owner=1) or shares it with another structure (owner=0). mem\_size is the number of elements the matrix can hold at most.

```
The following operations
                        are implemented on matrices and vectors.
                                                                       alpha
and beta are numbers,
                         A and B are matrices and x and y are vectors.
 pnl mat axpy
                                    B := alpha * A + B
 pnl mat scalar prod
 pnl mat dgemm
                                    C := alpha * op (A) * op (B) + beta * C
pnl_mat_mult_vect_transpose_inplace
                                    y = A' * x
pnl_mat_mult_vect_inplace
                                    y = A * x
pnl_mat_lAxpby
                                    y := alpha * A * x + beta * y
 pnl_mat_dgemv
                                    y := alpha * op (A) * x + beta * y
 pnl_mat_dger
                                    A := alpha x * y' + A
```

#### 4.3.2 Generic Functions

These functions exist for all types of matrices no matter what the basic type is. The following conventions are used to name functions operating on matrices. Here is the table of prefixes used for the different basic types.

type	prefix	BASE
double	pnl_mat	double
int	pnl_mat_int	int
dcomplex	pnl_mat_complex	dcomplex

In this paragraph we present the functions operating on PnlMat which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_mat and double according the above table.

Constructors and destructors There are no special functions to access the sizes of a matrix, instead the fields m, n and mn give direct access to the number of rows, columns and the size of the matrix.

- PnlMat \* pnl\_mat\_new ()
  Description Create a PnlMat of size 0
- PnlMat \* pnl\_mat\_create (int m, int n)

  Description Create a PnlMat with m rows and n columns.
- PnlMat \* pnl\_mat\_create\_from\_double (int m, int n, double x)

  Description Create a PnlMat with m rows and n columns and sets all the elements to x
- PnlMat \* pnl\_mat\_create\_from\_ptr (int m, int n, const double \*x)

  Description Create a PnlMat with m rows and n columns and copies the array x to the new vector. Be sure that x is long enough to fill all the vector because it cannot be checked inside the function.
- PnlMat \* pnl\_mat\_create\_from\_list (int m, int n, ...)

  Description Create a new PnlMat pointer of size m x n filled with the extra arguments passed to the function. The number of extra arguments passed must be equal to m x n, be aware that this cannot be checked inside the function.
- PnlMat \* pnl\_mat\_copy (const PnlMat \*M)

  Description Create a new PnlMat which is a copy of M.
- PnlMat \* pnl\_mat\_create\_diag\_from\_ptr (const double \*x, int d)
   Description Create a new squared PnlMat by specifying its size and diagonal terms as an array.
- PnlMat \* pnl\_mat\_create\_diag (const PnlVect \*V)

  Description Create a new squared PnlMat by specifying its diagonal terms in a PnlVect.
- PnlMat \* pnl\_mat\_create\_from\_file (const char \*file)

  Description Read a matrix from a file and creates the corresponding PnlMat. The following conventions are used for the storage in a file:
  - one row of the matrix corresponds to one line of the file
  - the elements of a row should be separated by blanks (spaces or tabs) and nothing else (no comma or semi-colon separators are detected).

- void pnl\_mat\_free (PnlMat \*\*M)
  Description Free a PnlMat and sets \*M to NULL
- PnlMat pnl\_mat\_wrap\_array (const double \*x, int m, int n)

  Description Create a PnlMat of size m x n which contains x. No copy is made. It is just a container.
- PnlMat pnl\_mat\_wrap\_vect (const PnlVect \*V)

  Description Return a PnlMat (not a pointer) whose array is the array of V. The new matrix shares its data with the vector V, which means that any modification to one of them will affect the other.
- void pnl\_mat\_clone (PnlMat \*clone, const PnlMat \*M)
   Description Clone M into clone. No no new PnlMat is created.
- int pnl\_mat\_resize (PnlMat \*M, int m, int n)

  Description Resize a PnlMat. The new matrix is of size m x n. The old data are lost.
- PnlVect \* pnl\_vect\_create\_submat (const PnlMat \*M, const PnlVectInt \*indi, const PnlVectInt \*indj)

  Description Create a new vector containing the values M(indi(:), indj(:)). indi and indj must be of the same size.
- void pnl\_vect\_extract\_submat (PnlVect \*V\_sub, const PnlMat \*M, const PnlVectInt \*indi, const PnlVectInt \*indj)

  Description On exit, V\_sub = M(indi(:), indj(:)). indi and indj must be of the same size.
- void pnl\_mat\_extract\_subblock (PnlMat \*M\_sub, const PnlMat \*M, int i, int len\_i, int j, int len\_j)

  Description M\_sub = M(i:i+len\_i-1, j:j+len\_j-1). len\_i (resp. len\_j) is the number of rows (resp. columns) to be extracted.

## Accessing elements

- void **pnl\_mat\_set** (**PnlMat** \*M, int i, int j, double x)
  Description Set the value of M[i, j]=x
- double **pnl\_mat\_get** (const **PnlMat** \*M, int i, int j) Description Get the value of M[i, j]
- double \* pnl\_mat\_lget (PnlMat \*M, int i, int j)

  Description Return the address of M[i, j] for use as a lvalue.
- void pnl\_mat\_set\_double (PnlMat \*M, double x)
  Description Set all elements of M to x.
- void **pnl\_mat\_set\_zero** (**PnlMat** \*M) Description Set all elements of M to 0.
- void pnl\_mat\_set\_id (PnlMat \*M)

  Description Set the matrix M to the identity matrix. M must be a square matrix.

- void **pnl\_mat\_set\_diag** (**PnlMat** \*M, double x, int d)

  Description Set the **d**<sup>th</sup> diagonal terms of the matrix M to the value x. M must be a square matrix.
- void pnl\_mat\_set\_from\_ptr (PnlMat \*M, const double \*x)

  Description Set M row—wise with the values given by x. The array x must be at least M->mn long.
- void **pnl\_mat\_get\_row** (PnlVect \*V, const PnlMat \*M, int i)

  Description Extract and copies the i-th row of M into V.
- void **pnl\_mat\_get\_col** (**PnlVect** \*V, const **PnlMat** \*M, int j) Description Extract and copies the j-th column of M into V.
- PnlVect pnl\_vect\_wrap\_mat\_row (const PnlMat \*M, int i)

  Description Return a PnlVect (not a pointer) whose array is the i-th row of M. The new vector shares its data with the matrix M, which means that any modification to one of them will affect the other.
- void **pnl\_mat\_swap\_rows** (**PnlMat** \*M, int i, int j) Description Swap two rows of a matrix.
- void pnl\_mat\_set\_col (PnlMat \*M, const PnlVect \*V, int j)

  Description Replace the i-th column of a matrix M by a vector V
- void **pnl\_mat\_set\_row** (PnlMat \*M, const PnlVect \*V, int i)

  Description Replace the i-th row of a matrix M by a vector V

Equivalently to the functions pnl\_mat\_get and pnl\_mat\_set, there exist macros for **PnlMat** only.

- MGET (M, i, j)

  Description Return M[i,j] for reading, eg. x=M(i,j)
- MLET (M, i, j)

  Description Return M[i,j] as a lvalue for writing, eg. eg. x=M(i,j)

## **Printing Matrices**

- void **pnl\_mat\_print** (const **PnlMat** \*M)

  Description Print a matrix to the standard output.
- void **pnl\_mat\_fprint** (FILE \*fic, const **PnlMat** \*M)

  Description Print a matrix to a file.
- void pnl\_mat\_print\_nsp (const PnlMat \*M)

  Description Print a matrix to the standard output in a format compatible with Nsp.
- void pnl\_mat\_fprint\_nsp (FILE \*fic, const PnlMat \*M)

  Description Print a matrix to a file in a format compatible with Nsp. The saved matrix can be reloaded by the function pnl mat create from file.

## Applying external operations

- void **pnl\_mat\_plus\_double** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar addition
- void **pnl\_mat\_minus\_double** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar substraction
- void **pnl\_mat\_mult\_double** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar multiplication
- void **pnl\_mat\_div\_double** (PnlMat \*lhs, double x)

  Description In-place matrix scalar division

## Element wise operations

- void pnl\_mat\_mult\_mat\_term (PnlMat \*lhs, const PnlMat \*rhs)

  Description In-place matrix matrix term by term product
- void **pnl\_mat\_div\_mat\_term** (**PnlMat** \*lhs, const **PnlMat** \*rhs)

  Description In-place matrix matrix term by term division
- void pnl\_mat\_map\_inplace (PnlMat \*lhs, double(\*f)(double))
  Description lhs = f(lhs).
- void pnl\_mat\_map (PnlMat \*lhs, const PnlMat \*rhs, double(\*f)(double))
  Description lhs = f(rhs).
- void pnl\_mat\_map\_mat\_inplace (PnlMat \*lhs, const PnlMat \*rhs, double(\*f)(double, double))

  Description lhs = f(lhs, rhs).
- void pnl\_mat\_map\_mat (PnlMat \*lhs, const PnlMat \*rhs1, const PnlMat \*rhs2, double(\*f)(double, double))

  Description lhs = f(rhs1, rhs2).
- double pnl\_mat\_sum (const PnlMat \*lhs)
   Description Sum matrix component-wise
- void pnl\_mat\_sum\_vect (PnlVect \*y, const PnlMat \*A, char c)

  Description Sum matrix column or row wise. Argument c can be either 'r' (to get a row vector) or 'c' (to get a column vector). When c='r',  $y(j) = \sum_i A_{ij}$  and when c='rc,  $y(i) = \sum_j A_{ij}$ .
- void pnl\_mat\_cumsum (PnlMat \*A, char c)

  Description Cumulative sum over the rows or columns. Argument c can be either 'r' to sum over the rows or 'c' to sum over the columns. When c='r',  $A_{ij}=\sum_{1\leq k\leq i}A_{kj}$  and when c='rc,  $A_{ij}=\sum_{1\leq k\leq j}A_{ik}$ .
- double pnl\_mat\_prod (const PnlMat \*lhs)
   Description Product matrix component-wise

- void pnl\_mat\_prod\_vect (PnlVect \*y, const PnlMat \*A, char c)
   Description Prod matrix column or row wise. Argument c can be either 'r' (to get a row vector) or 'c' (to get a column vector). When c='r', y(j) = ∏<sub>i</sub> A<sub>ij</sub> and when c='rc, y(i) = ∏<sub>i</sub> A<sub>ij</sub>.
- void pnl\_mat\_cumprod (PnlMat \*A, char c)

  Description Cumulative prod over the rows or columns. Argument c can be either 'r' to prod over the rows or 'c' to prod over the columns. When c='r',  $A_{ij}=\prod_{1\leq k\leq i}A_{kj}$  and when c='rc,  $A_{ij}=\prod_{1\leq k\leq j}A_{ik}$ .

#### Test functions

- int pnl\_mat\_eq (const PnlMat \*M1, const PnlMat \*M2)

  Description Test if two matrices are equal. Returns TRUE or FALSE.
- int pnl\_mat\_eq\_double (const PnlMat \*M, double x)

  Description Test if all the components of M are equal to x. Returns TRUE or FALSE.

## Ordering operations

- void  $pnl_mat_max$  ( pnlVect \*M, const pnlMat \*A, char d)

  Description On exit,  $M(i) = \max_j(A(i,j))$  when d='c' and  $M(i) = \max_j(A(j,i))$  when d='r' and  $M(0) = \max_{i,j} = A(i,j)$  when d='r'.
- void  $pnl_mat_min$  ( pnlVect \*m,const PnlMat \*A, char d)

  Description On exit,  $m(i) = \min_j(A(i,j))$  when d='c' and  $m(i) = \min_j(A(j,i))$  when d='r' and  $M(0) = \min_{i,j} = A(i,j)$  when d='r'.
- void  $\operatorname{pnl\_mat\_minmax}$  (  $\operatorname{PnlVect}$  \*m,  $\operatorname{PnlVect}$  \*M, const  $\operatorname{PnlMat}$  \*A, char d) Description On exit,  $\operatorname{m}(i) = \min_j(\operatorname{A}(i,j))$  and  $\operatorname{M}(i) = \max_j(\operatorname{A}(i,j))$  when  $\operatorname{d='c'}$  and  $\operatorname{m}(i) = \min_j(\operatorname{A}(j,i))$  and  $\operatorname{M}(i) = \min_j(\operatorname{A}(j,i))$  when  $\operatorname{d='r'}$  and  $\operatorname{M}(\operatorname{O}) = \max_{i,j} = \operatorname{A}(i,j)$  and  $\operatorname{m}(\operatorname{O}) = \min_{i,j} = \operatorname{A}(i,j)$  when  $\operatorname{d='*r'}$ .
- void pnl\_mat\_min\_index ( PnlVect \*m, PnlVectInt \*im, const PnlMat \*A, char d) Description Idem as pnl\_mat\_min and index contains the indices of the minima. If index==NULL, the indices are not computed.
- void pnl\_mat\_max\_index ( PnlVect \*M, PnlVectInt \*iM, const PnlMat \*A, char d)
   Description Idem as pnl\_mat\_max and index contains the indices of the maxima. If index==NULL, the indices are not computed.
- void pnl\_mat\_minmax\_index ( PnlVect \*m, PnlVect \*M, PnlVectInt \*im, PnlVectInt \*iM, const PnlMat \*A, char d)

  Description Idem as pnl\_mat\_minmax and im contains the indices of the minima and iM contains the indices of the minima. If im==NULL (resp. iM==NULL, the indices of the minima (resp. maxima) are not computed.
- void pnl\_mat\_qsort (PnlMat \*, char dir, char order)

  Description Sort a matrix using a quick sort algorithm according to order ('i' for

increasing or 'd' for decreasing). The parameter dir determines whether the matrix is sorted by rows or columns. If dir='c', each row is sorted independently of the others whereas if dir='r', each column is sorted independently of the others.

- void pnl\_mat\_qsort\_index (PnlMat \*, PnlMatInt \*index, char dir, char order)

  Description Sort a matrix using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing). The parameter dir determines whether the matrix is sorted by rows or columns. If dir='c', each row is sorted independently of the others whereas if dir='r', each column is sorted independently of the others. In addition to the function pnl\_mat\_qsort, the permutation index is computed and stored into index.
- int pnl\_mat\_find (PnlVectInt \*indi, PnlVectInt indj, char \*type, int(\*f)(double \*t), ...)

  Description f is a function taking a C array as argument and returning an integer. type

is a string composed by the letters 'r' and 'm' and is used to describe the types of the arguments appearing after f: 'r' for real numbers and 'm' for matrices. This function aims at simulating Scilab's find function. Here are a few examples (capital letters are used for matrices and small letters for real values)

```
- [indi, indj] = find ( a < X )
        int isless ( double *t ) { return t[0] < t[1]; }
        pnl_mat_find ( indi, indj, "rm", isless, a, X );

- ind = find (X <= Y)
        int isless ( double *t ) { return t[0] <= t[1]; }
        pnl_mat_find ( ind, "mm", isless, X, Y );

- [indi, indj] = find ((a < X) && (X <= Y))
        int cmp ( double *t )
        {
            return (t[0] <= t[1]) && (t[1] <= t[2]);
        }
        pnl_mat_find ( indi, indj, "rmm", cmp, a, X, Y );</pre>
```

(indi, indj) contains on exit the indices (i,j) for which the function f returned 1. Note that if indj == NULL on entry, a linear indexing is used for matrices, which means that matrices are seen as large vectors built up be stacking rows. This function returns OK or FAIL if something went wrong (size mismatch between matrices, invalid string type).

## Standard matrix operations

• void pnl\_mat\_plus\_mat (PnlMat \*lhs, const PnlMat \*rhs)

Description In-place matrix matrix addition

- void pnl\_mat\_minus\_mat (PnlMat \*lhs, const PnlMat \*rhs)
  Description In-place matrix matrix substraction
- void pnl\_mat\_sq\_transpose (PnlMat \*M)
  Description On exit, M is transposed
- PnlMat \* pnl\_mat\_transpose (const PnlMat \*M)

  Description Create a new matrix which is the transposition of M
- void pnl\_mat\_tr ( PnlMat \*tM, const PnlMat \*M)
   Description On exit, tM = M'
- void pnl\_mat\_axpy (double alpha, const PnlMat \*A, PnlMat \*B)
   Description Compute B := alpha \* A + B
- void pnl\_mat\_dger (double alpha, const PnlVect \*x, const PnlVect \*y, PnlMat \*A)

  Description Compute A := alpha x \* y' + A
- PnlVect \* pnl\_mat\_mult\_vect (const PnlMat \*A, const PnlVect \*x)

  Description Matrix vector multiplication A \* x
- void pnl\_mat\_mult\_vect\_inplace (PnlVect \*y, const PnlMat \*A, const PnlVect \*x)
   Description In place matrix vector multiplication y = A \* x. You cannot use the same vector for x and y.
- PnlVect \* pnl\_mat\_mult\_vect\_transpose (const PnlMat \*A, const PnlVect \*x)

  Description Matrix vector multiplication A' \* x
- void pnl\_mat\_mult\_vect\_transpose\_inplace (PnlVect \*y, const PnlMat \*A, const PnlVect \*x)
   Description In place matrix vector multiplication y = A' \* x. You cannot use the same vector for x and y. The vectors x and y must be different.
- int pnl\_mat\_cross (PnlMat \*lhs, const PnlMat \*A, const PnlMat \*B)

  Description Compute the cross products of the vectors given in matrices A and B which must have either 3 rows or 3 columns. A row wise computation is first tried, then a column wise approach is tested. FAIL is returned in case no dimension equals 3.
- void pnl\_mat\_lAxpby (double lambda, const PnlMat \*A, const PnlVect \*x, double mu, PnlVect \*b)
   Description Compute b := lambda A x + mu b. When mu==0, the content of b is not used on input and instead b is resized to match A\*x. The vectors x and b must be different.
- void pnl\_mat\_dgemv (char trans, double lambda, const PnlMat \*A, const PnlVect \*x, double mu, PnlVect \*b)
  Description Compute b := lambda op(A) x + mu b, where op (X) = X or op (X) = X'. If trans='N' or trans='n', op (A) = A, whereas if trans='T' or trans='t', op (A) = A'.When mu==0, the content of b is not used and instead b is resized to match op(A)\*x. The vectors x and b must be different.

- void pnl\_mat\_dgemm (char transA, char transB, double alpha, const PnlMat \*A, const PnlMat \*B, double beta, PnlMat \*C)

  Description Compute C := alpha \* op(A) \* op (B) + beta \* C. When beta=0, the content of C is unused and instead C is resized to store alpha A \*B. If transA='N' or transA='n', op (A) = A, whereas if transA='T' or transA='t', op (A) = A'. The same holds for transB. The matrix C must be different from A and B.
- PnlMat \* pnl\_mat\_mult\_mat (const PnlMat \*rhs1, const PnlMat \*rhs2)

  Description Matrix multiplication rhs1 \* rhs2
- void pnl\_mat\_mult\_mat\_inplace (PnlMat \*lhs, const PnlMat \*rhs1, const PnlMat \*rhs2)
   Description In-place matrix multiplication lhs = rhs1 \* rhs2. The matrix lhs must
- be different from rhs1 and rhs2.
  double pnl mat scalar prod (const PnlMat \*A, const PnlVect \*x, const PnlVect
- Description Compute x' \* A \* y
- void pnl\_mat\_exp (PnlMat \*B, const PnlMat \*A)

  Description Compute the matrix exponential B = exp(A).

Linear systems and matrix decompositions The following functions are designed to solve linear system of the from A x = b where A is a matrix and b is a vector except in the functions pnl\_mat\_syslin\_mat, pnl\_mat\_lu\_syslin\_mat and pnl\_mat\_chol\_syslin\_mat which expect the right hand side member to be a matrix too. Whenever the vector b is not needed once the system is solved, you should consider using "inplace" functions. All the functions described in this paragraph return OK if the computations have been carried out successfully and FAIL otherwise.

- int pnl\_mat\_chol (PnlMat \*M)
   Description Compute the Cholesky decomposition of M. M must be symmetric, the positivity is tested in the algorithm. M = L \* L'. On exit, the lower part of M contains the Cholesky decomposition L and the upper part is set to zero.
- int pnl\_mat\_pchol (PnlMat \*M, double tol, int \*rank, PnlVectInt \*p)
   Description Compute the Cholesky decomposition of M with complete pivoting. P' \* A \* P = L \* L'. M must be symmetric positive semi-definite. On exit, the lower part of M contains the Cholesky decomposition L and the upper part is set to zero. The permutation matrix is stored in an integer vector p: the only non zero elements of P are P(p(k),k) = 1
- int pnl\_mat\_lu (PnlMat \*A, PnlPermutation \*p)

  Description Compute a P A = LU factorization. P must be an already allocated PnlPermutation. On exit the decomposition is stored in A, the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1. Row i of A was interchanged with row p(i).
- int pnl\_mat\_upper\_syslin (PnlVect \*x, const PnlMat \*U, const PnlVect\*b)

  Description Solve an upper triangular linear system U x = b

- int pnl\_mat\_lower\_syslin (PnlVect \*x, const PnlMat \*L, const PnlVect\*b)

  Description Solve a lower triangular linear system L x = b
- int pnl\_mat\_chol\_syslin (PnlVect \*x, const PnlMat \*chol, const PnlVect \*b)

  Description Solve a symmetric definite positive linear system A x = b, in which chol is assumed to be the Cholesky decomposition of A computed by pnl mat chol
- int pnl\_mat\_chol\_syslin\_inplace (const PnlMat \*chol, PnlVect \*b)

  Description Solve a symmetric definite positive linear system A x = b, in which chol is assumed to be the Cholesky decomposition of A computed by pnl\_mat\_chol. The solution of the system is stored in b on exit.
- int pnl\_mat\_lu\_syslin (PnlVect \*x, const PnlMat \*LU, const PnlPermutation \*p, const PnlVect \*b)

  Description Solve a linear system A x = b using a LU decomposition. LU and P are assumed to be the PA = LU decomposition as computed by pnl\_mat\_lu. In particular, the structure of the matrix LU is the following: the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1.
- int pnl\_mat\_lu\_syslin\_inplace (const PnlMat \*LU, const PnlPermutation \*p, PnlVect \*b)

  Description Solve a linear system A x = b using a LU decomposition. LU and P are assumed to be the PA = LU decomposition as computed by pnl\_mat\_lu. In particular, the structure of the matrix LU is the following: the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1. The solution of the system is stored in b on exit.
- int pnl\_mat\_syslin (PnlVect \*x, const PnlMat \*A, const PnlVect \*b)

  Description Solve a linear system A x = b using a LU factorization which is computed inside this function.
- int pnl\_mat\_syslin\_inplace (PnlMat \*A, PnlVect \*b)

  Description Solve a linear system A x = b using a LU factorization which is computed inside this function. The solution of the system is stored in b and A is overwritten by its LU decomposition.
- int pnl\_mat\_syslin\_mat (PnlMat\*A, PnlMat \*B)
   Description Solve a linear system A X = B using a LU factorization which is computed inside this function. A and B are matrices. A must be square. The solution of the system is stored in B on exit. On exit, A contains the LU decomposition of the input matrix which is lost.
- int pnl\_mat\_chol\_syslin\_mat (const PnlMat\*A, PnlMat\*B)

  Description Solve a linear system A X = B using a Cholesky factorization of the symmetric positive definite matrix A. A contains the Cholesky decomposition as computed by pnl\_mat\_chol. B is matrix with the same number of rows as A. The solution of the system is stored in B on exit.

• int pnl\_mat\_lu\_syslin\_mat (const PnlMat\*A, const PnlPermutation \*p, PnlMat \*B)

Description Solve a linear system A X = B using a P A = L U factorization. A contains the L U factors and p the associated permutation. A and p must have been computed by pnl\_mat\_lu. B is matrix with the same number of rows as A. The solution of the system is stored in B on exit.

The following functions are designed to invert matrices. The authors provide these functions although they cannot find good reasons to use them. Note that to solve a linear system, one must used the syslin functions and not invert the system matrix because it is much longer.

- int pnl\_mat\_upper\_inverse (PnlMat \*A, const PnlMat \*B)

  Description Inversion of an upper triangular matrix
- int pnl\_mat\_lower\_inverse (PnlMat \*A, const PnlMat \*B)

  Description Inversion of a lower triangular matrix
- int pnl\_mat\_inverse (PnlMat \*inverse, const PnlMat \*A)

  Description Compute the inverse of a matrix A and stores the result into inverse. A

  LU factorisation of the matrix A is computed inside this function.
- int pnl\_mat\_inverse\_with\_chol (PnlMat \*inverse, const PnlMat \*A)

  Description Compute the inverse of a symmetric positive definite matrix A and stores the result into inverse. The Cholesky factorisation of the matrix A is computed inside this function.

# 4.3.3 Functions specific to base type double

## Standard matrix operations

- void pnl\_mat\_log (PnlMat \*B, const PnlMat \*A)

  Description Compute the matrix logarithm B = log(A). For the moment, this function only works if A is diagonalizable.
- void pnl\_mat\_eigen (PnlVect \*v, PnlMat \*P, const PnlMat \*A, int with\_eigenvector)
   Description Compute the eigenvalues (stored in v) and optionally the eigenvectors stored column wise in P when with\_eigenvector==TRUE. If A is symmetric, P is orthonormal.

Linear systems and matrix decompositions The following functions are designed to solve linear system of the from A x = b where A is a matrix and b is a vector except in the functions pnl\_mat\_syslin\_mat, pnl\_mat\_lu\_syslin\_mat and pnl\_mat\_chol\_syslin\_mat which expect the right hand side member to be a matrix too. Whenever the vector b is not needed once the system is solved, you should consider using "inplace" functions. All the functions described in this paragraph return OK if the computations have been carried out successfully and FAIL otherwise.

• int pnl\_mat\_qr (PnlMat \*Q, PnlMat \*R, PnlPermutation \*p, const PnlMat \*A) Description Compute a A P = QR decomposition. If on entry P=NULL, then the decomposition is computed without pivoting, i.e A = QR. When  $P \neq NULL$ , P must be an

already allocated PnlPermutation. Q is an orthogonal matrix, i.e  $Q^{-1} = Q^T$  and R is an upper triangular matrix. The use of pivoting improves the numerical stability when A is almost rank deficient, i.e when the smallest eigenvalue of A is very close to 0.

- int pnl\_mat\_qr\_syslin (PnlVect \*x, const PnlMat \*Q, const PnlMat \*R, const PnlVectInt \*p, const PnlVect \*b)

  Description Solve a linear system A x = b where A is given by its QR decomposition with column pivoting as computed by the function pnl\_mat\_qr.
- int pnl\_mat\_ls (const PnlMat\*A, PnlVect \*b)

  Description Solve a linear system A x = b in the least square sense, i.e.  $\mathbf{x} = \arg\min_{U} \|A*$   $u-b\|^2$ . The solution is stored into b on exit. It internally uses a AP = QR decomposition.
- int pnl\_mat\_ls\_mat (const PnlMat\*A, PnlMat\*B)

  Description Solve a linear system A X = B with A and B two matrices in the least square sense, i.e.  $X = \arg \min_{U} \|A*U B\|^2$ . The solution is stored into B on exit. It internally uses a AP = QR decomposition. Same function as pnl mat ls but handles several r.h.s.

#### 4.3.4 Permutations

typedef PnlVectInt PnlPermutation;

The PnlPermutation type is actually nothing else than a vector of integers, i.e. a PnlVectInt. It is used to store the partial pivoting with row interchanges transformation needed in the LU decomposition. We use the Blas convention for storing permutations. Consider a PnlPermutation p generated by a LU decomposition of a matrix A: to compute the decomposition, row i of A was interchanged with row p(i).

- PnlPermutation \* pnl\_permutation\_new ()
  Description Create an empty PnlPermutation.
- PnlPermutation \* pnl\_permutation\_create (int n) Description Create a PnlPermutation of size n.
- void **pnl\_permutation\_free** (PnlPermutation \*\*p) Description Free a PnlPermutation.
- void **pnl\_permutation\_inverse** (PnlPermutation\*inv, const PnlPermutation\*p)

  Description Compute in inv the inverse of the permutation p.
- void **pnl\_vect\_permute** (PnlVect \*px, const PnlVect \*x, const PnlPermutation \*p) Description Apply a PnlPermutation to a PnlVect.
- void pnl\_vect\_permute\_inplace (PnlVect \*x, const PnlPermutation \*p)

  Description Apply a PnlPermutation to a PnlVect in-place.
- void pnl\_vect\_permute\_inverse (PnlVect \*px, const PnlVect \*x, const PnlPermutation \*p)

  Description Apply the inverse of PnlPermutation to a PnlVect.

- void pnl\_vect\_permute\_inverse\_inplace (PnlVect \*x, const PnlPermutation \*p)

  Description Apply the inverse of a PnlPermutation to a PnlVect in-place.
- void pnl\_mat\_col\_permute (PnlMat \*pX, const PnlMat \*X, const PnlPermutation \*p)
   Description Apply a PnlPermutation to the columns of a matrix. pX contains the result of the permutation applied to X.
- void pnl\_mat\_row\_permute (PnlMat \*pX, const PnlMat \*X, const PnlPermutation \*p)
   Description Apply a PnlPermutation to the rows of a matrix. pX contains the result of the permutation applied to X.
- void **pnl\_permutation\_fprint** (FILE \*fic, const **PnlPermutation** \*p) Description Print a permutation to a file.
- void **pnl\_permutation\_print** (const **PnlPermutation** \*p) Description Print a permutation to the standard output.

# 4.4 Tridiagonal Matrices

#### 4.4.1 Overview

The structures and functions related to tridiagonal matrices are declared in pnl/pnl\_tridiag\_matrix.h.

We only store the three main diagonals as three vectors.

```
typedef struct PnlTridiagMat{
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlTridiagMat pointer to be cast to a PnlObject
    */
    PnlObject object;
    int size; /*!< number of rows, the matrix must be square */
    double *D; /*!< diagonal elements */
    double *DU; /*!< upper diagonal elements */
    double *DL; /*!< lower diagonal elements */
} PnlTridiagMat;</pre>
```

size is the size of the matrix, D is an array of size size containing the diagonal terms. DU, DL are two arrays of size size-1 containing respectively the upper diagonal  $(M_{i,i+1})$  and the lower diagonal  $(M_{i-1,i})$ .

```
typedef struct PnlTridiagMatLU{
   /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlTridiagMatLU pointer to be cast to a PnlObject
   */
PnlObject object;
```

```
int size; /*!< number of rows, the matrix must be square */
double *D; /*!< diagonal elements */
double *DU; /*!< upper diagonal elements */
double *DU2; /*!< second upper diagonal elements */
double *DL; /*!< lower diagonal elements */
int *ipiv; /*!< Permutation: row i has been interchanged with row ipiv(i) */
};</pre>
```

This type is used to store the LU decomposition of a tridiagonal matrix.

#### 4.4.2 Functions

#### Constructors and destructors

- PnlTridiagMat \* pnl\_tridiag\_mat\_new ()
  Description Create a PnlTridiagMat with size 0
- PnlTridiagMat \* pnl\_tridiag\_mat\_create (int size)
  Description Create a PnlTridiagMat with size size
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_double (int size, double x)
  Description Create a PnlTridiagMat with the 3 diagonals filled with x
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_two\_double (int size, double x, double y)

  Description Create a PnlTridiagMat with the diagonal filled with x and the upper and lower diagonals filled with y
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_ptr (int size, const double \*lower\_D, const double \*D, const double \*upper\_D)

  Description Create a PnlTridiagMat
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_mat (const PnlMat \*mat)

  Description Create a tridiagonal matrix from a full matrix (all the elements but the 3 diagonal ones are ignored).
- PnlMat \* pnl\_tridiag\_mat\_to\_mat (const PnlTridiagMat \*T)

  Description Create a full matrix from a tridiagonal one.
- PnlTridiagMat \* pnl\_tridiag\_mat\_copy (const PnlTridiagMat \*T) Description Copy a tridiagonal matrix.
- void pnl\_tridiag\_mat\_clone (PnlTridiagMat \*clone, const PnlTridiagMat \*T)

  Description Copy the content of T into clone
- void pnl\_tridiag\_mat\_free (PnlTridiagMat \*\*v)
  Description Free a PnlTridiagMat
- int pnl\_tridiag\_mat\_resize (PnlTridiagMat \*v, int size)
  Description Resize a PnlTridiagMat.

## Accessing elements

- void pnl\_tridiag\_mat\_set (PnlTridiagMat \*self, int d, int up, double x)
   Description Set self[d, d+up] = x, up can be {-1,0,1}.
- double **pnl\_tridiag\_mat\_get** (const **PnlTridiagMat** \*self, int d, int up) Description Get self[d, d+up], up can be {-1,0,1}.
- double \* pnl\_tridiag\_mat\_lget (PnlTridiagMat \*self, int d, int up)

  Description Return the address self[d, d+up] = x, up can be {-1,0,1}.

# **Printing Matrix**

- void **pnl\_tridiag\_mat\_fprint** (FILE \*fic, const **PnlTridiagMat** \*M)

  Description Print a tri-diagonal matrix to a file.
- void **pnl\_tridiag\_mat\_print** (const **PnlTridiagMat** \*M)

  Description Print a tridiagonal matrix to the standard output.

## Algebra operations

- void pnl\_tridiag\_mat\_plus\_tridiag\_mat (PnlTridiagMat \*lhs, const PnlTridiag-Mat \*rhs)
   Description In-place matrix matrix addition
- void pnl\_tridiag\_mat\_minus\_tridiag\_mat (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs)
   Description In-place matrix matrix substraction
- void **pnl\_tridiag\_mat\_plus\_double** (**PnlTridiagMat** \*lhs, double x) Description In-place matrix scalar addition
- void **pnl\_tridiag\_mat\_minus\_double** (**PnlTridiagMat** \*lhs, double x) Description In-place matrix scalar substraction
- void **pnl\_tridiag\_mat\_mult\_double** (**PnlTridiagMat** \*lhs, double x)

  Description In-place matrix scalar multiplication
- void **pnl\_tridiag\_mat\_div\_double** (**PnlTridiagMat** \*lhs, double x)

  Description In-place matrix scalar division

## Element-wise operations

- void pnl\_tridiag\_mat\_mult\_tridiag\_mat\_term (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs)

  Description In-place matrix matrix term by term product
- void pnl\_tridiag\_mat\_div\_tridiag\_mat\_term (PnlTridiagMat \*lhs, const Pnl-TridiagMat \*rhs)

  Description In-place matrix matrix term by term division

- void **pnl\_tridiag\_mat\_map\_inplace** (**PnlTridiagMat** \*lhs, double(\*f)(double))

  Description lhs = f(lhs).
- void pnl\_tridiag\_mat\_map\_tridiag\_mat\_inplace (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs, double(\*f)(double, double))

  Description lhs = f(lhs, rhs).

# Standard matrix operations & Linear systems

- void pnl\_tridiag\_mat\_mult\_vect\_inplace (PnlVect \*lhs, const PnlTridiagMat \*mat, const PnlVect \*rhs)

  Description In place matrix multiplication. The vector 1hs must be different from rhs.
- PnlVect \* pnl\_tridiag\_mat\_mult\_vect (const PnlTridiagMat \*mat, const PnlVect \*vec)

  Description Matrix multiplication
- void pnl\_tridiag\_mat\_lAxpby (double lambda, const PnlTridiagMat \*A, const PnlVect \*x, double mu, PnlVect \*b)

  Description Compute b := lambda A x + mu b. When mu==0, the content of b is not used on input and instead b is resized to match A\*x. Note that the vectors x and b must be different.
- double pnl\_tridiag\_mat\_scalar\_prod (const PnlVect \*x,const PnlTridiagMat \*A, const PnlVect \*y)
   Description Compute x' \* A \* y
- void pnl\_tridiag\_mat\_syslin\_inplace ( PnlTridiagMat \*M, PnlVect \*b) Description Solve the linear system M = b. The solution is written into b on exit. On exit, M is modified and becomes unusable.
- void  $pnl\_tridiag\_mat\_syslin$  (PnlVect \*x, PnlTridiagMat \*M, const PnlVect \*b) Description Solve the linear system M x = b. On exit, M is modified and becomes unusable.
- PnlTridiagMatLU\* pnl\_tridiag\_mat\_lu\_new ()
  Description Create an empty PnlTridiagMatLU
- PnlTridiagMatLU\* pnl\_tridiag\_mat\_lu\_create (int size)
  Description Create a PnlTridiagMatLU with size size
- PnlTridiagMatLU\* pnl\_tridiag\_mat\_lu\_copy (const PnlTridiagMatLU \*mat) Description Create a new PnlTridiagMatLU which is a copy of mat.
- void pnl\_tridiag\_mat\_lu\_clone (PnlTridiagMatLU \*clone, const PnlTridiag-MatLU \*mat)

  Description Clone a PnlTridiagMatLU. clone must already exist, no memory is allocated for the envelope.
- void pnl\_tridiag\_mat\_lu\_free (PnlTridiagMatLU \*\*m)
  Description Free a PnlTridiagMatLU

- int pnl\_tridiag\_mat\_lu\_resize (PnlTridiagMatLU \*v, int size) Description Resize a PnlTridiagMatLU
- int pnl\_tridiag\_mat\_lu\_compute (PnlTridiagMatLU \*LU, const PnlTridiagMat \*A)

  Description Compute the LU factorisation of a tridiagonal matrix A. LU must have already been created using pnl\_tridiag\_mat\_lu\_new. On exit, LU contains the decomposition which is suitable for use in pnl\_tridiag\_mat\_lu\_syslin.
- int pnl\_tridiag\_mat\_lu\_syslin\_inplace (PnlTridiagMatLU \*LU, PnlVect \*b)

  Description Solve a linear system A x = b where the matrix LU is given the LU decomposition of A previously computed by pnl\_tridiag\_mat\_lu\_compute. On exit, b is overwritten by the solution x.
- int pnl\_tridiag\_mat\_lu\_syslin (PnlVect \*x, PnlTridiagMatLU \*LU, const PnlVect \*b)

  Description Solve a linear system A x = b where the matrix LU is given the LU decomposition of A previously computed by pnl\_tridiag\_mat\_lu\_compute.

## 4.5 Band Matrices

#### 4.5.1 Overview

```
typedef struct
{
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlBandMat pointer to be cast to a PnlObject
    */
PnlObject object;
int m; /*!< nb rows */
int n; /*!< nb columns */
int nu; /*!< nb of upperdiagonals */
int nl; /*!< nb of lowerdiagonals */
int m_band; /*!< nb rows of the band storage */
int n_band; /*!< nb columns of the band storage */
double *array; /*!< a block to store the bands */
} PnlBandMat;</pre>
```

The structures and functions related to band matrices are declared in pnl/pnl\_band\_matrix.h.

#### 4.5.2 Functions

#### Constructors and destructors

• PnlBandMat\* pnl\_band\_mat\_new ()
Description Create a band matrix of size 0.

- PnlBandMat\* pnl\_band\_mat\_create (int m, int n, int nl, int nu)

  Description Create a band matrix of size m x n with nl lower diagonals and nu upper diagonals.
- PnlBandMat\* pnl\_band\_mat\_create\_from\_mat (const PnlMat \*BM, int nl, int nu)

  Description Extract a band matrix from a PnlMat.
- void pnl\_band\_mat\_free (PnlBandMat\*\*)
  Description Free a band matrix.
- void pnl\_band\_mat\_clone (PnlBandMat \*clone, const PnlBandMat \*M)

  Description Copy the band matrix M into clone. No new PnlBandMat is created.
- PnlBandMat\* pnl\_band\_mat\_copy (PnlBandMat \*BM)

  Description Create a new band matrix which is a copy of BM. Each band matrix owns its data array.
- PnlMat\* pnl\_band\_mat\_to\_mat (PnlBandMat \*BM)
  Description Create a full matrix from a band matrix.
- int pnl\_band\_mat\_resize (PnlBandMat \*BM, int m, int n, int nl, int nu)

  Description Resize BM to store a m x n band matrix with nu upper diagonals and nl lower diagonals.

## Accessing elements

- void pnl\_band\_mat\_set (PnlBandMat \*M, int i, int j, double x) Description  $M_{i,j} = x$ .
- void  $pnl\_band\_mat\_get$  (PnlBandMat \*M, int i, int j) Description Return  $M_{i,j}$ .
- void pnl\_band\_mat\_lget (PnlBandMat \*M, int i, int j) Description Return the address & $(M_{i,j})$ .
- void **pnl\_band\_mat\_set\_double** (**PnlBandMat** \*M, double x) Description Set all the elements of M to x.
- void pnl\_band\_mat\_print\_as\_full (PnlBandMat \*M)

  Description Print a band matrix in a full format.

# Element wise operations

- void pnl\_band\_mat\_plus\_double (PnlBandMat \*lhs, double x)
  Description In-place addition, 1hs += x
- void pnl\_band\_mat\_minus\_double (PnlBandMat \*lhs, double x)
   Description In-place substraction lhs -= x
- void pnl\_band\_mat\_div\_double (PnlBandMat \*lhs, double x)
   Description lhs = lhs ./ x

- void pnl\_band\_mat\_mult\_double (PnlBandMat \*lhs, double x)
  Description lhs = lhs \* x
- void pnl\_band\_mat\_plus\_band\_mat (PnlBandMat \*lhs, const PnlBandMat \*rhs)

Description In-place addition, lhs += rhs

• void **pnl\_band\_mat\_minus\_band\_mat** (**PnlBandMat** \*lhs, const **PnlBandMat** \*rhs)

Description In-place substraction lhs -= rhs

- void pnl\_band\_mat\_inv\_term (PnlBandMat \*lhs)
   Description In-place term by term inversion lhs = 1 ./ rhs
- void pnl\_band\_mat\_div\_band\_mat\_term (PnlBandMat \*lhs, const PnlBand-Mat \*rhs)

Description In-place term by term division lhs = lhs ./ rhs

void pnl\_band\_mat\_mult\_band\_mat\_term (PnlBandMat \*lhs, const PnlBand-Mat \*rhs)

Description In-place term by term multiplication lhs = lhs .\* rhs

- void pnl\_band\_mat\_map (PnlBandMat \*lhs, const PnlBandMat \*rhs, double(\*f)(double))

  Description lhs = f(rhs)
- $\bullet \ \ \mathrm{void} \ \mathbf{pnl\_band\_mat\_map\_inplace} \ (\underline{PnlBandMat} \ *lhs, \ \mathrm{double}(*f)(\mathrm{double}))$
- void pnl\_band\_mat\_map\_band\_mat\_inplace (PnlBandMat \*lhs, const Pnl-BandMat \*rhs, double(\*f)(double,double))

  Description lhs = f(lhs,rhs)

# Standard matrix operations & Linear system

Description lhs = f(lhs)

- void pnl\_band\_mat\_lAxpby (double lambda, const PnlBandMat \*A, const PnlVect \*x, double mu, PnlVect \*b)
   Description Compute b := lambda A x + mu b. When mu==0, the content of b is not used on input and instead b is resized to match the size of A\*x.
- void pnl\_band\_mat\_mult\_vect\_inplace (PnlVect \*y, const PnlBandMat \*BM, const PnlVect \*x)
   Description y = BM \* x
- void pnl\_band\_mat\_syslin\_inplace (PnlBandMat \*M, PnlVect \*b)

  Description Solve the linear system M x = b with M a PnlBandMat. Note that M is modified on output and becomes unusable. On exit, the solution x is stored in b.
- void pnl\_band\_mat\_syslin (PnlVect \*x,PnlBandMat \*M, PnlVect \*b)

  Description Solve the linear system M x = b with M a PnlBandMat. Note that M is modified on output and becomes unusable.

- void pnl\_band\_mat\_lu (PnlBandMat \*BM, PnlVectInt \*p)

  Description Compute the LU decomposition with partial pivoting with row interchanges.

  On exit, BM is enlarged to store the LU decomposition. On exit, p stores the permutation applied to the rows. Note that the Lapack format is used to store p, this format differs from the one used by PnlPermutation.
- void pnl\_band\_mat\_lu\_syslin\_inplace (const PnlBandMat \*M, PnlVectInt \*p, PnlVect \*b)

  Description Solve the band linear system M x = b where M is the LU decomposition computed by pnl\_band\_mat\_lu and p the associated permutation. On exit, the solution x is stored in b.
- void pnl\_band\_mat\_lu\_syslin (PnlVect \*x, const PnlBandMat \*M, PnlVectInt \*p, const PnlVect \*b)
   Description Solve the band linear system M x = b where M is the LU decomposition computed by pnl\_band\_mat\_lu and p the associated permutation.

# 4.6 Hyper Matrices

# 4.6.1 Short description

The Hyper matrix types and related functions are defined in the header pnl/pnl\_matrix.h.

```
typedef struct PnlHmat{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlHmat pointer to be cast to a PnlObject
  PnlObject object;
  int ndim; /*!< nb dimensions */
  int *dims; /*!< pointer to store the values of the ndim dimensions */
  int mn; /*!< product dim_1 *...*dim_ndim */</pre>
  int *pdims; /*!< array of size ndim, s.t. pdims[i] = dims[ndim-1] x ... dims[i+1]</pre>
                with pdims[ndim - 1] = 1 */
  double *array; /*!< pointer to store */</pre>
} PnlHmat;
typedef struct PnlHmatInt{
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlHmatInt pointer to be cast to a PnlObject
   */
  PnlObject object;
  int ndim; /*!< nb dimensions */
  int *dims; /*!< pointer to store the value of the ndim dimensions */
  int mn; /*!< product dim_1 *...*dim_ndim */</pre>
  int *pdims; /*!< array of size ndim, s.t. pdims[i] = dims[ndim-1] x ... dims[i+1]
                with pdims[ndim - 1] = 1 */
```

ndim is the number of dimensions, dim is an array to store the size of each dimension and nm contains the product of the sizes of each dimension. array is an array of size mn containing the data. The integer array pdims is used to create the one—to—one map between the natural indexing and the linear indexing used in array.

## 4.6.2 Generic Functions

**General functions** These functions exist for all types of hypermatrices no matter what the basic type is. The following conventions are used to name functions operating on hypermatrices. Here is the table of prefixes used for the different basic types.

$_{\mathrm{type}}$	prefix	BASE
double	pnl_hmat	double
int	$pnl\_hmat\_int$	int
dcomplex	pnl_hmat_complex	dcomplex

In this paragraph, we present the functions operating on PnlHmat which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_hmat and double according the above table.

#### 4.6.3 Functions

#### Constructors and destructors

- PnlHmat \* pnl\_hmat\_new ()
  Description Create an empty PnlHmat.
- PnlHmat \* pnl\_hmat\_create (int ndim, const int \*dims)

  Description Create a PnlHmat with ndim dimensions and the size of each dimension is given by the entries of the integer array dims
- PnlHmat \* pnl\_hmat\_create\_from\_double (int ndim, const int \*dims, double x) Description Create a PnlHmat with ndim dimensions given by  $\prod_i \text{dims}[i]$  filled with x.

- PnlHmat \* pnl\_hmat\_create\_from\_ptr (int ndim, const int \*dims, const double \*x)
- void **pnl\_hmat\_free** (PnlHmat \*\*H)
  Description Free a PnlHmat
- PnlHmat \* pnl\_hmat\_copy (const PnlHmat \*H)
  Description Copy a PnlHmat.
- void pnl\_hmat\_clone (PnlHmat \*clone, const PnlHmat \*H)

  Description Clone a PnlHmat.
- int pnl\_hmat\_resize (PnlHmat \*H, int ndim, const int \*dims)
  Description Resize a PnlHmat.

## Accessing elements

- void **pnl\_hmat\_set** (**PnlHmat** \*self, int \*tab, double x) Description Set the element of index tab to x.
- double pnl\_hmat\_get (const PnlHmat \*self, int \*tab)

  Description Return the value of the element of index tab
- double\* pnl\_hmat\_lget (PnlHmat \*self, int \*tab)

  Description Return the address of self[tab] for use as a lvalue.
- PnlMat pnl\_mat\_wrap\_hmat (PnlHmat \*H, int \*t)

  Description Return a true PnlMat not a pointer holding the data H(t,:,:). Note that t must be of size ndim-2 and that it cannot be checked within the function. The returned matrix shares its data with H, it is only a view not a true copy.
- PnlVect pnl\_vect\_wrap\_hmat (PnlHmat \*H, int \*t)

  Description Return a true PnlVect not a pointer holding the data H(t,:). Note that t must be of size ndim-1 and that it cannot be checked within the function. The returned vector shares its data with H, it is only a view not a true copy.

## Printing hypermatrices

• void **pnl\_hmat\_print** (const **PnlHmat** \*H) Description Print an hypermatrix.

## Term by term operations

- void pnl\_hmat\_plus\_hmat (PnlHmat \*lhs, const PnlHmat \*rhs)
  Description Compute lhs += rhs.
- void **pnl\_hmat\_mult\_double** (**PnlHmat** \*lhs, double x)

  Description Compute **lhs** \*= x where x is a real number.

## 4.7 Iterative Solvers

#### 4.7.1 Overview

The structures and functions related to solvers are declared in pnl/pnl\_linalgsolver.h.

```
typedef struct _PnlIterationBase PnlIterationBase;
typedef struct _PnlCgSolver PnlCgSolver;
typedef struct _PnlBicgSolver PnlBicgSolver;
typedef struct PnlGmresSolver PnlGmresSolver;
struct _PnlIterationBase
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlVectXXX pointer to be cast to a PnlObject
  PnlObject object;
  int iteration;
  int max_iter;
  double normb;
  double tol_;
  double resid;
  int error;
  /* char * err_msg; */
};
/* When you repeatedly use iterative solvers, do not malloc each time */
struct _PnlCgSolver
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlCgSolver pointer to be cast to a PnlObject
  PnlObject object;
  PnlVect * r;
  PnlVect * z;
  PnlVect * p;
  PnlVect * q;
  double rho;
  double oldrho;
  double beta;
  double alpha;
  PnlIterationBase * iter;
} ;
struct _PnlBicgSolver
{
```

```
/**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlBicgSolver pointer to be cast to a PnlObject
  PnlObject object;
  double rho_1, rho_2, alpha, beta, omega;
  PnlVect * p;
  PnlVect * phat;
  PnlVect * s;
  PnlVect * shat;
  PnlVect * t;
  PnlVect * v;
  PnlVect * r;
  PnlVect * rtilde;
  PnlIterationBase * iter;
} ;
struct _PnlGmresSolver
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlGmresSolver pointer to be cast to a PnlObject
  PnlObject object;
  int restart;
  double beta;
  PnlVect * s;
  PnlVect * cs;
  PnlVect * sn;
  PnlVect * w;
  PnlVect * r;
  PnlMat * H;
  PnlVect * v[MAX_RESTART];
  PnlIterationBase *iter;
  PnlIterationBase *iter_inner;
};
```

A Left preconditioner solves the problem :

$$PMx = Pb$$
,

and whereas right preconditioner solves

$$MPy = b, \qquad Py = x.$$

More information is given in Saad, Yousef (2003). Iterative methods for sparse linear systems (2nd ed. ed.). SIAM. ISBN 0898715342. OCLC 51266114. The reader will find in this book some discussion about right or/and left preconditioner and a description of the following algorithms.

These algorithms, we implemented with a left preconditioner. Right preconditioner can be easily computed changing matrix vector multiplication operator from M x to M  $P_R$  x and solving  $P_R y = x$  at the end of algorithm.

#### 4.7.2 Functions

Three methods are implemented: Conjugate Gradient, BICGstab and GMRES with restart. For each of them a structure is created to store temporary vectors used in the algorithm. In some cases, we have to apply iterative methods more than once: for example to solve at each time step a discrete form of an elliptic problem come from parabolic problem. In the cases, do not call the constructor and destructor at each time, but instead use the initialization and solve procedures.

Formally we have,

```
Create iterative method

For each time step
   Initialisation of iterative method
   Solve linear system link to elliptic problem
end for
free iterative method
```

In these functions, we don't use any particular matrix structure. We give the matrix vector multiplication as a parameter of the solver.

Conjugate Gradient method Only available for symmetric and positive matrices.

- PnlCgSolver \* pnl\_cg\_solver\_new ()
  Description Create an empty PnlCgSolver
- PnlCgSolver \* pnl\_cg\_solver\_create (int Size, int max-iter, double tolerance)
  Description Create a new PnlCgSolver pointer.
- void pnl\_cg\_solver\_initialisation (PnlCgSolver \*Solver, const PnlVect \*b)

  Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_cg\_solver\_free (PnlCgSolver \*\*Solver)

  Description Destructor of iterative solver
- int pnl\_cg\_solver\_solve (void(\*matrix vector-product)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlCgSolver \*Solver)

  Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditionner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

## **BICG** stab

PnlBicgSolver \* pnl\_bicg\_solver\_new ()
 Description Create an empty PnlBicgSolver.

- PnlBicgSolver \* pnl\_bicg\_solver\_create (int Size, int max-iter, double tolerance)
  Description Create a new PnlBicgSolver pointer.
- void pnl\_bicg\_solver\_initialisation (PnlBicgSolver \*Solver, const PnlVect \*b)

  Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_bicg\_solver\_free (PnlBicgSolver \*\*Solver)

  Description Destructor of iterative solver
- int pnl\_bicg\_solver\_solve (void(\*matrix vector-product)(const void \*, const Pn-lVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlBicgSolver \*Solver)

  Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditioner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

**GMRES** with restart See Saad, Yousef (2003) for a discussion about the restart parameter. For GMRES we need to store at the p-th iteration p vectors of the same size of the right and side. It could be very expensive in term of memory allocation. So GMRES with restart algorithm stop if p = restart and restarts the algorithm with the previously computed solution as initial guess.

Note that if restart equals m, we have a classical GMRES algorithm.

- PnlGmresSolver \* pnl\_gmres\_solver\_new ()
  Description Create an empty PnlGmresSolver
- PnlGmresSolver \* pnl\_gmres\_solver\_create (int Size, int max-iter, int restart, double tolerance)
   Description Create a new PnlGmresSolver pointer.
- void pnl\_gmres\_solver\_initialisation (PnlGmresSolver \*Solver, const PnlVect \*b)

  Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_gmres\_solver\_free (PnlGmresSolver \*\*Solver)
  Description Destructor of iterative solver
- int pnl\_gmres\_solver\_solve (void(\*matrix vector-product)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlGmresSolver \*Solver)

  Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditionner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

In the next paragraph, we write all the solvers for PnlMat. This will be done as follows: construct an application matrix vector.

In practice, we cannot define all iterative methods for all structures. With this implementation, the user can easily :

- implement right precondioner,
- implement method with sparse matrix and diagonal preconditioner, or special combination of this form . . .

# Iterative algorithms for PnlMat

- int pnl\_mat\_cg\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, const PnlVect \*b, PnlCgSolver \*Solver)

  Description Solve the linear system M x = b with preconditionner PC.
- int pnl\_mat\_bicg\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, const PnlVect \*b, PnlBicgSolver \*Solver)
   Description Solve the linear system M x = b with preconditionner PC.
- int pnl\_mat\_gmres\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, PnlVect \*b, PnlGmresSolver \*Solver)

  Description Solve the linear system M x = b with preconditionner PC.

#### 5 Cumulative distribution Functions

The functions related to this chapter are declared in pnl/pnl\_cdf.h.

For various distribution functions, we provide functions named pnl\_cdf\_xxx where xxx is the

abbreviation of the distribution name. All these functions are based on the same prototype

$$p = 1 - q; \quad p = \int_{-\infty}^{\infty} density(u) du$$

- which If which=1, it computes p and q. If which=2, it computes x. For higher values of which it computes one the parameters characterizing the distribution using all the others, p, q, x.
- p the probability  $\int_{0}^{x} density(u) du$
- q = 1 p

- x the upper bound of the integral
- status an integer which indicates on exit the success of the computation. (0) if calculation completed correctly. (-I) if the input parameter number I was out of range. (1) if the answer appears to be lower than the lowest search bound. (2) if the answer appears to be higher than the greatest search bound. (3) if  $p + q \neq 1$ .
- bound is undefined if STATUS is 0. Bound exceeded by parameter number I if STATUS is negative. Lower search bound if STATUS is 1. Upper search bound if STATUS is 2.
- void **pnl\_cdf\_bet** (int \*which, double \*p, double \*q, double \*x, double \*y, double \*a, double \*b, int \*status, double \*bound)

  Description Cumulative Distribution Function BETA distribution.
- void **pnl\_cdf\_bin** (int \*which, double \*p, double \*q, double \*x, double \*xn, double \*pr, double \*ompr, int \*status, double \*bound)

  Description Cumulative Distribution Function BINa distribution.
- void **pnl\_cdf\_chi** (int \*which, double \*p, double \*q, double \*x, double \*df, int \*status, double \*bound)

  Description Cumulative Distribution Function CHI-Square distribution.
- void **pnl\_cdf\_chn** (int \*which, double \*p, double \*q, double \*x, double \*df, double \*pnonc, int \*status, double \*bound)

  Description Cumulative Distribution Function Non-central Chi-Square distribution.
- void **pnl\_cdf\_f** (int \*which, double \*p, double \*q, double \*x, double \*dfn, double \*dfd, int \*status, double \*bound)

  Description Cumulative Distribution Function F distribution.
- void **pnl\_cdf\_fnc** (int \*which, double \*p, double \*q, double \*x, double \*dfn, double \*dfd, double \*pnonc, int \*status, double \*bound)

  Description Cumulative Distribution Function Non-central F distribution.
- void **pnl\_cdf\_gam** (int \*which, double \*p, double \*q, double \*x, double \*shape, double \*scale, int \*status, double \*bound)

  Description Cumulative Distribution Function GAMma distribution.
- void **pnl\_cdf\_nbn** (int \*which, double \*p, double \*q, double \*x, double \*xn, double \*pr, double \*ompr, int \*status, double \*bound)

  Description Cumulative Distribution Function Negative BiNomial distribution.
- void pnl\_cdf\_nor (int \*which, double \*p, double \*q, double \*x, double \*mean, double \*sd, int \*status, double \*bound)
   Description Cumulative Distribution Function NORmal distribution.
- void **pnl\_cdf\_poi** (int \*which, double \*p, double \*q, double \*x, double \*xlam, int \*status, double \*bound)

  Description Cumulative Distribution Function POIsson distribution.

- void **pnl\_cdf\_t** (int \*which, double \*p, double \*q, double \*x, double \*df, int \*status, double \*bound)
  - Description Cumulative Distribution Function T distribution.
- double pnl\_cdfchi2n (double x, double df, double ncparam)
   Description Compute the cumulative density function at x of the non central χ² distribution with df degrees of freedom and non centrality parameter ncparam.
- void pnl\_cdfbchi2n (double x, double df, double ncparam, double beta, double \*P)
   Description Store in P the cumulative density function at x of the random variable beta \*X where X is non central χ² random variable with df degrees of freedom and non centrality parameter ncparam.
- double **pnl\_normal\_density** (double x) Description Normal density function.
- double **pnl\_cdfnor** (double x)

  Description Cumulative normal distribution function.
- double **pnl\_cdf2nor** (double a, double b, double r)

  Description Cumulative bivariate normal distribution function, returns  $\frac{1}{2\pi\sqrt{1-r^2}} \int_{-\infty}^a \int_{-\infty}^b e^{-\frac{x^2-2rxy+y^2}{2(1-r^2)}} dxdy.$
- double **pnl\_inv\_cdfnor** (double x)

  Description Inverse of the cumulative normal distribution function.

# 6 Random Number Generators

The functionalities described in this chapter are declared in pnl/pnl\_random.h.

Random number generators should be called through the new *rng* interface based on the PnlRng object. This interface uses reentrant functions and is suitable for multi-threaded applications.

The older *rand* interface is kept for compatibility issues only and hould not be used in newly written code.

# 6.1 The rng interface

It is possible to create random number generators each with its own state variable so that they can evolve independently in a shared memory environment. These generators are suitable for use in multi-threaded programs.

Random generator	index	Type	Info
KNUTH	PNL_RNG_KNUTH	pseudo	
MRGK3	PNL_RNG_MRGK3	pseudo	
MRGK5	PNL_RNG_MRGK5	pseudo	
SHUFL	PNL_RNG_SHUFL	pseudo	
L'ECUYER	PNL_RNG_L_ECUYER	pseudo	
TAUSWORTHE	PNL_RNG_TAUSWORTHE	pseudo	
MERSENNE	PNL_RNG_MERSENNE	pseudo	
SQRT	PNL_RNG_SQRT	quasi	
HALTON	PNL_RNG_HALTON	quasi	
FAURE	PNL_RNG_FAURE	quasi	
SOBOL_I4	PNL_RNG_SOBOL_I4	quasi	uses 32 bit intergers
SOBOL_I8	PNL_RNG_SOBOL2_I8	quasi	uses 64 bit intergers
NIEDERREITER	PNL_RNG_NIEDERREITER	quasi	

Table 2: Indices of the random generators

```
int rand_or_quasi; /*!< can be PNL_MC or PNL_QMC */
int dimension; /*!< dimension of the space in which we draw the samples */
int counter; /*!< counter = number of samples already drawn */
int has_gauss; /*!< Is a gaussian deviate available? */
double gauss; /*!< If has_gauss==1, gauss a gaussian sample */
int size_state; /*!< size in bytes of the state variable */
void *state; /*!< state of the random generator */
};</pre>
```

- void pnl\_rng\_free (PnlRng \*\*)
  Description Free a PnlRng.
- PnlRng\* pnl\_rng\_create (int type)

  Description Create a PnlRng corresponding to type which can be any of the values

  PNL\_RNG\_XXX listed in Table 2 which correspond to pseudo random number generators.

  Once a generator has been created, you must call pnl\_rng\_sseed before using it.
- void pnl\_rng\_sseed (PnlRng \*rng, unsigned long int s)

  Description Set the seed of the genrator rng using s. If s=0, then a default seed (depending on the generator) is used.
- int pnl\_rng\_sdim (PnlRng \*rng, int dim)

  Description Set the dimension of the state space for a QMC generator and initializes it accordingly. Returns OK if the generator has been initialized properly and FAIL otherwise.
- PnlRng\* pnl\_rng\_copy (const PnlRng \*rng)
  Description Create a copy of rng.
- void pnl\_rng\_clone (PnlRng \*dest, const PnlRng \*src)

  Description Copy the content of src into the already existing basis dest. On exit, src and dest are identical but independent.

- PnlRng\* pnl\_rng\_dcmt\_create\_id (int id, ulong seed)

  Description Create a generator with type PNL\_RNG\_DCMT and identifier id. Two generators with different ids are independent. Note that the returned generator must be initialized with pnl\_rng\_sseed before usage. The identifier id can for instance correspond to the thread number or the processor rank in parallel computing.
- PnlRng\*\* pnl\_rng\_dcmt\_create\_array\_id (int start\_id, int max\_id, ulong seed, int \*count)
   Description Create an array of generators with types PNL\_RNG\_DCMT and identifiers linearly varying between start\_id and max\_id. The number of generators created is max\_id start\_id + 1. All the generators are independent. Note that each generator of the returned array must be initialized with pnl\_rng\_sseed before usage.
- PnlRng \*\* pnl\_rng\_dcmt\_create\_array (int n, ulong seed, int \*count)

  Description Create an array of n independent DCMT. seed is the seed used to initialize the Mersenne Twister generator internally used to find new DCMT. On exit, count contains the number of generators actually created. Same function as pnl\_dcmt\_create\_array instead that it directly returns an array of PnlRng. Before using the generators, you must initialize each of them by calling the function pnl\_rng\_sseed count times.

Some auxiliary functions internally used (to use with caution)

- PnlRng\* pnl\_rng\_new ()
  Description Create an empty PnlRng.
- void pnl\_rng\_init (PnlRng \*rng, int type)

  Description Initialize an empty PnlRng as returned by pnl\_rng\_new to become a generator of type type which can be any of the values PNL\_RNG\_XXX listed in Table 2 which correspond to pseudo random number generators. Calling pnl\_rng\_create is equivalent to calling first pnl\_rng\_new and then pnl\_rng\_init.
- PnlRng\* pnl\_rng\_get\_from\_id (int id)

  Description Return the global generator described by its macro name. The variable id can be any of the values PNL\_RNG\_XXX listed in Table 2.

The following functions return one sample from a specified law.

- int pnl\_rng\_bernoulli (double p, PnlRng \*rng)

  Description Generate a sample from the Bernouilli law on {0,1} with parameter p.
- long pnl\_rng\_poisson (double lambda, PnlRng \*rng)

  Description Generate a sample from the Poisson law with parameter lambda.
- double pnl\_rng\_exp (double lambda, PnlRng \*rng)

  Description Generate a sample from the Exponential law with parameter lambda.
- double **pnl\_rng\_uni** (PnlRng \*rng)

  Description Generate a sample from the Uniform law on [0, 1].
- double  $pnl\_rng\_uni\_ab$  (double a, double b, PnlRng \*rng)

  Description Generate a sample from the Uniform law on [a, b].

- double pnl\_rng\_normal (PnlRng \*rng)

  Description Generate a sample from the standard normal distribution.
- long pnl\_rng\_poisson1 (double lambda, double t, PnlRng \*rng)

  Description Generate a sample from a Poisson process with intensity lambda at time t.
- double pnl\_rng\_gamma (double a, double b, PnlRng \*rng) Description Generate a sample from the  $\Gamma(a, b)$  distribution.
- double pnl\_rng\_chi2 (double n, PnlRng \*rng) Description Generate a sample from the centered  $\chi^2(n)$  distribution.
- double pnl\_rng\_bessel (double v, double a,PnlRng \*rng)
   Description Generate a sample from the Bessel distribution with parameters v > -1 and a > 0.
- double pnl\_rng\_gauss (int d, int create\_or\_retrieve, int index, PnlRng \*rng)

  Description The second argument can be either CREATE (to actually draw the sample)
  or RETRIEVE (to retrieve that element of index index). With CREATE, it draws d random normal variables and stores them for future usage. They can be withdrawn using
  RETRIEVE with the index of the number to be retrieved.

The following functions take an already existing PnlVect\*as its first argument and fill each entry of the vector with a sample from the specified law. All the entries are independent. The difference between n-samples from a distribution in dimension 1, and one sample from the same distribution in dimension n only matters when using a **Quasi** random number generator.

- void **pnl\_vect\_rng\_uni** (PnlVect \*G, int samples, double a, double b, PnlRng \*rng) Description G is a vector of independent and identically distributed samples from the uniform distribution on [a, b].
- void pnl\_vect\_rng\_normal (PnlVect \*G, int samples, PnlRng \*rng)
   Description G is a vector of independent and identically distributed samples from the standard normal distribution.
- void  $pnl\_vect\_rng\_uni\_d$  (PnlVect \*G, int d, double a, double b, PnlRng \*rng) Description G is a sample from the uniform distribution on  $[a, b]^d$ .
- void pnl\_vect\_rng\_normal\_d (PnlVect \*G, int d, PnlRng \*rng)

  Description G is a sample from the d-dimensional standard normal distribution.

The following functions take an already existing PnlMat\*as first argument and fill each entry of the vector with a sample from the specified law. All the entries are in-dependant. On return, the matrix M is of size samples x dimension. The rows of M are independently and identically distributed. Each row is a sample from the given law in dimension dimension.

- void pnl\_mat\_rng\_uni (PnlMat \*M, int samples, int d, const PnlVect \*a, const PnlVect \*b, PnlRng \*rng)

  Description M contains samples samples from the uniform distribution on  $\prod_{i=1}^{d} [a_i, b_i]$ .
- void pnl\_mat\_rng\_uni2 (PnlMat \*M, int samples, int d, double a, double b, PnlRng \*rng)

  Description M contains samples samples from the uniform distribution on  $[a, b]^d$ .

• void pnl\_mat\_rng\_normal (PnlMat \*M, int samples, int d, PnlRng \*rng)

Description M contains samples samples from the d-dimensional standard normal distribution.

```
Some examples
#include <stdlib.h>
#include "pnl/pnl_random.h"
int main ()
  int i, M;
  PnlRng *rng = pnl_rng_create (PNL_RNG_MERSENNE);
  PnlVect *v = pnl_vect_new ();
  M = 10000;
  /* rng must be initialized. When sseed=0, a default
     value depending on the generator is used */
     pnl_rng_sseed (rng, 0);
  for ( i=0 ; i<M ; i++ )
    /* Simulates a normal random vector in R^{10} */
    pnl_vect_rng_normal (v, 10, rng);
    /* Do something with v */
  pnl_vect_free (&v);
  pnl_rng_free (&rng); /* Frees the generator */
  exit(0);
}
#include <stdlib.h>
#include <time.h>
#include "pnl/pnl_random.h"
int main ()
{
  int i, M;
  double E;
  PnlRng *rng = pnl_rng_create (PNL_RNG_MERSENNE);
  M = 10000;
  /* rng must be initialized. */
  rng = pnl_rng_sseed (time (NULL));
  for ( i=0 ; i<M ; i++ )
```

{

```
/* Simulates an exponential random variable */
E = pnl_rng_exp (1, rng);
/* Do something with E */
}

pnl_rng_free (&rng); /* Frees the generator */
exit (0);
}
```

# 6.2 The *rand* interface (deprecated)

**Note**: For backward compatibility with older versions of the PNL, we still provide the old rand interface to random number generation although we strongly encourage users to use the new rng interface (see section 6.1).

Every generator is identified by an integer valued macro. One must **NOT** refer to a generator using directly the value of the macro PNL\_RNG\_XXX because there is no warranty that the order used to store the generators will remain the same in future releases. Instead, one should call generators directly using their macro names.

The initial seeds of all the generators are fixed by the function pnl\_rand\_init but you can change it by calling pnl\_rand\_sseed.

Before starting to use random number generators, you must initialize them by calling

- int pnl\_rand\_init (int type\_generator, int simulation\_dim, long samples)

  Description It resets the sample counter to 0 and checks that the generator described by type\_generator can actually generate samples in dimension simulation\_dim and fixes the seed.
- int pnl\_rand\_or\_quasi (int type\_generator)

  Description Return the type the generator of index type\_generator, PNL\_MC or PNL\_
  QMC
- void pnl\_rand\_sseed ((int type\_generator, unsigned long int seed))
   Description It sets the seed of the generator type\_generator with seed.
- const char \* pnl\_rand\_name (int type\_generator)

  Description Return the name of the generator of index type\_generator

Once a generator is chosen, there are several functions available in the library to draw samples according to a given law.

The following functions return one sample from a specified law.

- int pnl\_rand\_bernoulli (double p, int type\_generator)

  Description Generate a sample from the Bernouilli law on {0,1} with parameter p.
- long pnl\_rand\_poisson (double lambda, int type\_generator)

  Description Generate a sample from the Poisson law with parameter lambda.
- double **pnl\_rand\_exp** (double lambda, int type\_generator)

  Description Generate a sample from the Exponential law with parameter lambda.

- double **pnl\_rand\_uni** (int type\_generator)

  Description Generate a sample from the Uniform law on [0, 1].
- double  $pnl\_rand\_uni\_ab$  (double a, double b, int type\\_generator) Description Generate a sample from the Uniform law on [a, b].
- double **pnl\_rand\_normal** (int type\_generator)

  Description Generate a sample from the standard normal distribution.
- long pnl\_rand\_poisson1 (double lambda, double t, int type\_generator)

  Description Generate a sample from a Poisson process with intensity lambda at time t.
- double **pnl\_rand\_gamma** (double a, double b, int type\_generator) Description Generate a sample from the  $\Gamma(a,b)$  distribution.
- double pnl\_rand\_chi2 (double n, int type\_generator) Description Generate a sample from the centered  $\chi^2(n)$  distribution.
- double pnl\_rand\_bessel (double v, double a, int generator) Description Generate a sample from the Bessel distribution with parameters v > -1 and a > 0.

The following functions take an already existing PnlVect\* as its first argument and fill each entry of the vector with a sample from the specified law. All the entries are independent. The difference between n-samples from a distribution in dimension 1, and one sample from the same distribution in dimension n only matters when using a **Quasi** random number generator.

- void pnl\_vect\_rand\_uni (PnlVect \*G, int samples, double a, double b, int type\_generator)
   Description G is a vector of independent and identically distributed samples from the uniform distribution on [a, b].
- void pnl\_vect\_rand\_normal (PnlVect \*G, int samples, int generator)
   Description G is a vector of independent and identically distributed samples from the standard normal distribution.
- void **pnl\_vect\_rand\_uni\_d** (**PnlVect** \*G, int d, double a, double b, int type\_generator)

  Description G is a sample from the uniform distribution on  $[a,b]^d$ .
- void pnl\_vect\_rand\_normal\_d (PnlVect \*G, int d, int generator)

  Description G is a sample from the d-dimensional standard normal distribution.

The following functions take an already existing PnlMat\* as first argument and fill each entry of the vector with a sample from the specified law. All the entries are in-dependent. On return, the matrix M is of size samples x dimension. The rows of M are independently and identically distributed. Each row is a sample from the given law in dimension dimension.

• void pnl\_mat\_rand\_uni (PnlMat \*M, int samples, int d, const PnlVect \*a, const PnlVect \*b, int type\_generator)

Description M contains samples samples from the uniform distribution on  $\prod_{i=1}^{d} [a_i, b_i]$ .

- void **pnl\_mat\_rand\_uni2** (**PnlMat** \*M, int samples, int d, double a, double b, int type\_generator)

  Description M contains samples samples from the uniform distribution on [a, b]<sup>d</sup>.
- void **pnl\_mat\_rand\_normal** (**PnlMat** \*M, int samples, int d, int type\_generator)

  Description M contains **samples** samples from the d-dimensional standard normal distribution.

Because of the use of **Quasi** random number generators, you may need to draw a set of samples at once because they represent one sample from a multi-dimensional distribution. The following function enables to draw one sample from the **dimension**-dimensional standard normal distribution and store it so that you can access the elements individually afterwards.

double pnl\_rand\_gauss (int d, int create\_or\_retrieve, int index, int type\_generator)
 Description The second argument can be either CREATE (to actually draw the sample)
 or RETRIEVE (to retrieve that element of index index). With CREATE, it draws d random normal variables and stores them for future usage. They can be withdrawn using
 RETRIEVE with the index of the number to be retrieved.

# 6.2.1 Advanced usage

We also provide functions for directly manipulating Mersenne Twister and "Dynamically created Mersenne Twister" random number generators, although we believe one should rather use the new *rng* interface.

Mersenne Twister It is possible to create Mersenne Twister random number generators each with its state variable.

```
typedef struct
{
  unsigned long mt[624];
  int mti;
} mt_state;
typedef unsigned long ulong;
```

- void **pnl\_mt\_sseed** (mt\_state \*state, unsigned long int s)

  Description Set the initial value of variable **state** using **s**
- ulong pnl\_mt\_genrand (mt\_state \*state)

  Description Return the following number in the sequence as an unsigned long variable.

  A mask is applied so that only the lowest 32-bits are used.
- double pnl\_mt\_genrand\_double (mt\_state \*state)

  Description Return the following number in the sequence as a double.

Dynamically created Mersenne Twister These are Mersenne Twister type generators with Mersenne exponent fixed to p=521 and word length w=32 bits. These choices are hard coded and cannot be changed without altering the code directly.

```
typedef struct
{
  ulong aaa;
  int mm,nn,rr,ww;
  ulong wmask,umask,lmask;
  int shift0, shift1, shiftB, shiftC;
  ulong maskB, maskC;
  int i;
  ulong state[17];
} dcmt_state;
```

Some functions to use "Dynamically Created Mersenne Twister" random number generators (DCMT).

- dcmt\_state\* pnl\_dcmt\_get\_parameter (ulong seed)

  Description Create a DCMT. seed is the seed used to initialize the Mersenne Twister generator internally used to find new DCMT.
- dcmt\_state \*\* pnl\_dcmt\_create\_array (int n, ulong seed, int \*count)

  Description Create an array of n independent DCMT. seed is the seed used to initialize the Mersenne Twister generator internally used to find new DCMT. On exit, count contains the number of generators actually created.
- double **pnl\_dcmt\_genrand\_double** (dcmt\_state \*mts)

  Description Generate a uniformly distributed random variable on [0,1].
- void **pnl\_dcmt\_free** (dcmt\_state \*\*mts)

  Description Free a dcmt.
- void **pnl\_dcmt\_free\_array** (dcmt\_state \*\*mts, int count)

  Description Free an array of dcmt as returned by pnl\_dcmt\_create\_array

# 7 Function bases and regression

#### 7.1 Overview

To use these functionalities, you should include pnl/pnl\_basis.h.

```
struct PnlBasis_t {
  int
  const char *label; /*!< string to label the basis *</pre>
              nb_variates; /*!< number of variates *
  int
  int
              nb_func; /*!< number of elements in the basis *
  PnlMatInt *T; /*!< Tensor matrix *</pre>
  double
            (*f)(double
                          x, int i); /*!< Computes the i-th element
                                       of the one dimensional basis */
  double
            (*Df)(double x, int i); /*!< Computes the first derivative
                   of the i-th element of the one dimensional basis */
            (*D2f)(double x, int i); /*! < Computes the second derivative
  double
```

Table 3: Names of the bases. See also function pnl\_basis\_type\_register to register more basis types.

In this section, we provide functions to solve regression problems on finite dimensional bases. Let  $(x_i, i = 1...n)$  be n points in  $\mathbb{R}^d$  and a function g defined by the data  $(y_i = g(x_i), i = 1...n)$ . Assume you want to approximate the function g by its decomposition on a family of N functions  $(f_j, j = 1...N)$ . Then, we want to compute the vector  $\alpha^* \in \mathbb{R}^N$  solving

$$\alpha^* = \arg\min_{\alpha} \sum_{i=1}^n \left( \sum_{j=0}^N \alpha_j f_j(x_i) - y_i \right)^2$$

## 7.2 Functions

• int pnl\_basis\_type\_register (const char \*name, double (\*f)(double, int), double (\*Df)(double, int), double (\*D2f)(double, int))

Description Register a new basis type and return the index to be passed to pnl\_basis\_create. The variable name is a unique string identifier of the family. The variables f, Df, D2f are the one dimensional basis functions, its first and second order derivatives. Each of these functions must return a double and take two arguments: the first one is the point at which evaluating the basis functions, the second one is the index of function. Here is a toy example to show how the canonical basis is registered (this family is actually already available with the id PNL\_BASIS\_CANONICAL, so the following example may look a little fake)

```
double f(double x, int n) { return pnl_pow_i(x, n); }
double Df(double x, int n) { return n * pnl_pow_i(x, n-1); }
double f(double x, int n) { return n * (n-1) * pnl_pow_i(x, n-2); }
int id = pnl_basis_register ("Canonic", f, Df, D2f);
/*
   * B is the Canonical basis of polynomials with degree less or equal than 2 in  
   * dimension 5.
   */
PnlBasis *B = pnl_basis_create_from_degree (id, 2, 5);
```

- PnlBasis \* pnl\_basis\_new ()
  Description Create an empty PnlBasis.
- void pnl\_basis\_print (const PnlBasis \*B)

  Description Print the characteristics of a basis.
- PnlBasis \* pnl\_basis\_create (int index, int nb\_func, int nb\_variates)

  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with nb\_variates variates. The basis will contain nb\_func.
- PnlBasis \* pnl\_basis\_create\_from\_degree (int index, int degree, int nb\_variates)

  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with total degree less or equal than degree and nb\_variates variates. The total degree is the sum of the partial degrees.

  For instance, calling pnl\_basis\_create, from degree (index, 2, 4) is equivalent to

For instance, calling pnl\_basis\_create\_from\_degree (index, 2, 4) is equivalent to calling pnl\_basis\_create\_from\_tensor (index, T) where T is given by

$$\left(\begin{array}{ccccc}
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & 0 & 1 \\
0 & 0 & 1 & 1 \\
2 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 \\
0 & 0 & 2 & 0 \\
0 & 0 & 0 & 2
\end{array}\right)$$

- PnlBasis \* pnl\_basis\_create\_from\_prod\_degree (int index, int degree, int nb\_variates)

  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with total degree less or equal than degree and nb\_variates variates. The total degree is the product of MAX(1, d\_i) where the d\_i are the partial degrees.
- PnlBasis \* pnl\_basis\_create\_from\_tensor (int index, PnlMatInt \*T)

  Description Create a PnlBasis for the polynomial family defined by index (see Table 3) using the basis described by the tensor matrix T. The number of lines of T is the number of functions of the basis whereas the numbers of columns of T is the number of variates of the functions. Note that T is not copied inside this function but only its address is stored, so never free T. It will be freed when calling pnl\_basis\_free on the returned object. i

Here is an example of a tensor matrix. Assume you are working with three variate

functions, the basis { 1, x, y, z,  $x^2$ , xy, yz,  $z^3$ } is decomposed in the one dimensional canonical basis using the following tensor matrix

$$\begin{pmatrix}
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
2 & 0 & 0 \\
1 & 1 & 0 \\
0 & 1 & 1 \\
0 & 0 & 3
\end{pmatrix}$$

- void pnl\_basis\_clone (PnlBasis \*dest, const PnlBasis \*src)

  Description Clone src into dest. The basis dest must already exist before calling this function. On exit, dest and src are identical and independent.
- PnlBasis\* pnl\_basis\_copy (const PnlBasis \*B)
  Description Create a copy of B.
- void pnl\_basis\_set\_from\_tensor (PnlBasis \*b, int index, const PnlMatInt \*T)

  Description Set an alredy existing basis b to a polynomial family defined by index (see Table 3) using the basis described by the tensor matrix T. The number of lines of T is the number of functions of the basis whereas the numbers of columns of T is the number of variates of the functions.
  - Same function as pnl\_basis\_create\_from\_tensor except that it operates on an already existing basis.
- PnlBasis\* pnl\_basis\_create\_from\_hyperbolic\_degree (int index, double degree, double q, int n)

  Description Create a sparse basis of polynomial with n variates. We give the example of the Canonical basis. A canonical polynomial with n variates writes  $X_1^{\alpha_1}X_2^{\alpha_2}...X_n^{\alpha_n}$ . To be a member of the basis, it must satisfy  $(\sum_{i=1}^n \alpha_i^q)^{1/q} \leq degree$ . This kind of basis based on an hyperbolic set of indices gives priority to polynomials associated to low order interaction.
- void pnl\_basis\_free (PnlBasis \*\*basis)

  Description Free a PnlBasis created by pnl\_basis\_create. Beware that basis is the address of a PnlBasis\*.

Functional regression based on a least square approach often leads to ill conditioned linear systems. One way of improving the stability of the system is to use centered and renormalised polynomials so that the original domain of interest  $\mathcal{D}$  (a subset of  $\mathbb{R}^d$ ) is mapped to  $[-1,1]^d$ . If the domain  $\mathcal{D}$  is rectangular and writes [a,b] where  $a,b \in \mathbb{R}^d$ , the mapping is done by

$$x \in \mathcal{D} \longmapsto \left(\frac{x_i - (b_i + a_i)/2}{(b_i - a_i)/2}\right)_{i=1,\dots,d}$$
 (1)

• void pnl\_basis\_set\_domain (PnlBasis \*B, const PnlVect \*a, const PnlVect \*b)

Description This function declares B as a centered and normalised basis as defined by

Equation 1. Calling this function is equivalent to calling pnl\_basis\_set\_reduced with

center=(b+a)/2 and scale=(b-a)/2.

• void pnl\_basis\_set\_reduced (PnlBasis \*B, const PnlVect \*center, const PnlVect \*scale)

Description This function declares B as a centered and normalised basis using the mapping

$$x \in \mathcal{D} \longmapsto \left( \frac{x_i - \mathtt{center}_i}{\mathtt{scale}_i} \right)_{i=1,\cdots,d}$$

• int pnl\_basis\_fit\_ls (PnlBasis \*P, PnlVect \*coef, PnlMat \*x, PnlVect \*y)

Description Compute the coefficients coef defined by

$$coef = \arg\min_{\alpha} \sum_{i=1}^{n} \left( \sum_{j=0}^{N} \alpha_{j} P_{j}(x_{i}) - y_{i} \right)^{2}$$

where N is the number of functions to regress upon and n is the number of points at which the values of the original function are known.  $P_j$  is the j-th basis function. Each row of the matrix x defines the coordinates of one point  $x_i$ . The function to be approximated is defined by the vector y of the values of the function at the points x.

- double **pnl\_basis\_ik\_vect** (const **PnlBasis** \*b, const **PnlVect** \*x, int i, int k) Description An element of a basis writes  $\prod_{l=0}^{\text{nb}_{v}\text{ariates}} \phi_l(x_l)$  where the  $\phi$ 's are one dimensional polynomials. This functions computes the therm  $\phi_k$  of the i-th basis function at the point x.
- double **pnl\_basis\_i\_vect** (const **PnlBasis** \*b, const **PnlVect** \*x, int i) Description If b is composed of  $f_0, \ldots, f_{nb \text{ func}-1}$ , then this function returns  $f_i(x)$ .
- double **pnl\_basis\_i\_D\_vect** (const **PnlBasis** \*b, const **PnlVect** \*x, int i, int j) Description If b is composed of  $f_0, \ldots, f_{nb\_func-1}$ , then this function returns  $\partial_{x_j} f_i(x)$ .
- double pnl\_basis\_i\_D2\_vect (const PnlBasis \*b, const PnlVect \*x, int i, int j1, int j2)

  Description If b is composed of  $f_0, \ldots, f_{nb\_func-1}$ , then this function returns  $\partial^2_{x_{j1}, x_{j2}} f_i(x)$ .
- void pnl\_basis\_eval\_derivs\_vect (const PnlBasis \*b, const PnlVect \*coef, const PnlVect \*x, double \*fx, PnlVect \*Dfx, PnlMat \*D2fx)
   Description Compute the function, the gradient and the Hessian matrix of ∑<sub>k=0</sub><sup>n</sup> coef<sub>k</sub>P<sub>k</sub>(·) at the point x. On output, fx contains the value of the function, Dfx its gradient and D2fx its Hessian matrix. This function is optimized and performs much better than calling pnl\_basis\_eval, pnl\_basis\_eval\_D and pnl\_basis\_eval\_D2 sequentially.
- double pnl\_basis\_eval\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x)

  Description Compute the linear combination of P\_k(x) defined by coef. Given the coefficients computed by the function pnl\_basis\_fit\_ls, this function returns  $\sum_{k=0}^{n} \operatorname{coef}_{k} P_{k}(\mathbf{x})$ .
- double pnl\_basis\_eval\_D\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x, int i)

Description Compute the derivative with respect to  $x_i$  of the linear combination of  $P_k(x)$  defined by coef. Given the coefficients computed by the function pnl\_basis\_-fit\_ls, this function returns  $\partial_{x_i} \sum_{k=0}^{n} \operatorname{coef}_k P_k(x)$  The index i may vary between 0 and P->nb\_variates - 1.

- double pnl\_basis\_eval\_D2\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x, int i, int j)

  Description Compute the derivative with respect to x\_i of the linear combination of P\_k(x) defined by coef. Given the coefficients computed by the function pnl\_basis\_fit\_ls, this function returns  $\partial_{x_i}\partial_{x_j}\sum_{k=0}^n \operatorname{coef}_k P_k(x)$ . The indices i and j may vary between 0 and P->nb\_variates 1.
- double **pnl\_basis\_ik** (const **PnlBasis** \*b, const double \*x, int i, int k)

  Description Same as function pnl\_basis\_ik\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_i** (**PnlBasis** \*b, double \*x, int i)

  Description Same as function pnl\_basis\_i\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_i\_D ( const PnlBasis \*b, const double \*x, int i, int j )

  Description Same as function pnl\_basis\_i\_D\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_i\_D2** (const **PnlBasis** \*b, const double \*x, int i, int j1, int j2) Description Same as function pnl\_basis\_i\_D2\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_eval** (PnlBasis \*P, PnlVect\*coef, double \*x)

  Description Same as function pnl\_basis\_eval\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_eval\_D** (**PnlBasis** \*P, **PnlVect** \*coef, double \*x, int i)

  Description Same as function pnl\_basis\_eval\_D\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_eval\_D2 (PnlBasis \*P, PnlVect \*coef, double \*x, int i, int j)

  Description Same as function pnl\_basis\_eval\_D2\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_eval\_derivs (PnlBasis \*P, PnlVect\*coef, double \*x, double \*fx, PnlVect \*Dfx, PnlMat \*D2fx)
   Description Same as function pnl\_basis\_eval\_derivs\_vect but takes a C array as the point of evaluation.

# 8 Numerical integration

#### 8.1 Overview

To use these functionalities, you should include pnl/pnl\_integration.h.

Numerical integration methods are designed to numerically evaluate the integral over a finite or non finite interval (resp. over a square) of real valued functions defined on  $\mathbb{R}$  (resp. on  $\mathbb{R}^2$ ).

```
typedef struct {
  double (*function) (double x, void *params);
  void *params;
} PnlFunc;

typedef struct {
  double (*function) (double x, double y, void *params);
  void *params;
} PnlFunc2D;

We provide the following two macros to evaluate a PnlFunc or PnlFunc2D at a given point
#define PNL_EVAL_FUNC(F, x) (*((F)->function))(x, (F)->params)
#define PNL_EVAL_FUNC2D(F, x, y) (*((F)->function))(x, y, (F)->params)
```

#### 8.2 Functions

- double pnl\_integration (PnlFunc \*F, double x0, double x1, int n, char \*meth) Description Evaluate  $\int_{x_0}^{x_1} F$  using n discretization steps. The method used to discretize the integral is defined by meth which can be "rect" (rectangle rule), "trap" (trapezoidal rule), "simpson" (Simpson's rule).
- double pnl\_integration\_2d (PnlFunc2D \*F, double x0, double x1, double y0, double y1, int nx, int ny, char \*meth)

  Description Evaluate  $\int_{[x_0,x_1]\times[y_0,y_1]}F$  using nx (resp. ny) discretization steps for [x0, x1] (resp. [y0, y1]). The method used to discretize the integral is defined by meth which can be "rect" (rectangle rule), "trap" (trapezoidal rule), "simpson" (Simpson's rule).
- int pnl\_integration\_qng (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

  Description Evaluate  $\int_{x_0}^{x_1} F$  with an absolute error less than espabs and a relative error less than esprel. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of function evaluations. This function returns 0K if the required accuracy has been reached and FAIL otherwise. This function uses a non-adaptive Gauss Konrod procedure (qng routine from QuadPack).
- int pnl\_integration\_GK (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

  Description This function is a synonymous of pnl\_integration\_qng and is only available for backward compatibility. It is deprecated, please use pnl\_integration\_qng instead.
- int pnl\_integration\_qng\_2d (PnlFunc2D \*F, double x0, double x1, double y0, double y1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

Description Evaluate  $\int_{[x_0,x_1]\times[y_0,y_1]} F$  with an absolute error less than espabs and a relative error less than esprel. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of function evaluations. This function returns OK if the required accuracy has been reached and FAIL otherwise.

- int pnl\_integration\_GK2D (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

  Description This function is a synonymous of pnl\_integration\_qng\_2d and is only available for backward compatibility. It is deprecated, please use pnl\_integration\_qng\_2d instead.
- int pnl\_integration\_qag (PnlFunc \*F, double x0, double x1, double epsabs, int limit, double epsrel, double \*result, double \*abserr, int \*neval)

  Description Evaluate  $\int_{x_0}^{x_1} F$  with an absolute error less than espabs and a relative error less than esprel. x0 and x1 can be non finite (i.e. PNL\_NEGINF or PNL\_POSINF). The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of iterations. limit is the maximum number of subdivisions of the interval (x0,x1) used during the integration. If on input, limit 0, then 750 subdivisions are used. This function returns 0K if the required accuracy has been reached and FAIL otherwise. This function uses some adaptive procedures (qags and qagi routines from QuadPack). This function is able to handle functions F with integrable singularities on the interval [x0,x1].
- int pnl\_integration\_qagp (PnlFunc \*F, double x0, double x1, const PnlVect \*singularities, double epsabs, int limit, double epsrel, double \*result, double \*abserr, int \*neval)

  Description Evaluate  $\int_{x_0}^{x_1} F$  for a function F with known singularities listed in singularities. singularities must be a sorted vector which does not contain x0 nor x1. x0 and x1 must be finite. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of iterations. limit is the maximum number of subdivisions of the interval (x0,x1) used during the integration. If on input, limit = 0, then 750 subdivisions are used. This function returns 0K if the required accuracy has been reached and FAIL otherwise. This function uses some adaptive procedures (qagp routine from QuadPack). This function is able to handle functions F with integrable singularities on the interval [x0,x1].

# 9 Fast Fourier Transform

#### 9.1 Overview

The forward Fourier transform of a vector c is defined by

$$z_j = \sum_{k=1}^{N} c_k e^{-i(j-1)(k-1)2\pi/N}, \quad j = 1, \dots, N$$

The inverse Fourier transform enables to recover c from z and is defined by

$$c_k = \sum_{j=1}^{N} z_j e^{i(j-1)(k-1)2\pi/N}, \quad j = 1, \dots, N$$

The coefficients of the Fourier transform of a real function satisfy the following relation

$$z_k = \overline{z_{N-k}},\tag{2}$$

where N is the number of discretization points.

A few remarks on the FFT of real functions and its inverse transform:

- We only need half of the coefficients.
- When a value is known to be real, its imaginary part is not stored. So the imaginary part of the zero-frequency component is never stored as it is known to be zero.
- For a sequence of even length the imaginary part of the frequency n/2 is not stored either, since the symmetry (2) implies that this is purely real too.

**FFTPack storage** The functions use the fftpack storage convention for half-complex sequences. In this convention, the half-complex transform of a real sequence is stored with frequencies in increasing order, starting from zero, with the real and imaginary parts of each frequency in neighboring locations.

The storage scheme is best shown by some examples. The table below shows the output for an odd-length sequence, n=5. The two columns give the correspondence between the 5 values in the half-complex sequence (stored in a PnlVect V) and the values (PnlVectComplex C) that would be returned if the same real input sequence were passed to pnl\_dft\_complex as a complex sequence (with imaginary parts set to 0),

$$C(0) = V(0) + i0,$$

$$C(1) = V(1) + iV(2),$$

$$C(2) = V(3) + iV(4),$$

$$C(3) = V(3) - iV(4) = \overline{C(2)},$$

$$C(4) = V(1) + iV(2) = \overline{C(1)}$$
(3)

The elements of index greater than N/2 of the complex array, as C(3) C(4), are filled in using the symmetry condition.

The next table shows the output for an even-length sequence, n = 6. In the even case there are two values which are purely real,

$$C(0) = V(0) + i0,$$

$$C(1) = V(1) + iV(2),$$

$$C(2) = V(3) + iV(4),$$

$$C(3) = V(5) - i0 = \overline{C(0)},$$

$$C(4) = V(3) - iV(4) = \overline{C(2)},$$

$$C(5) = V(1) + iV(2) = \overline{C(1)}$$

$$(4)$$

#### 9.2 Functions

To use the following functions, you should include pnl/pnl\_fft.h.

The following functions comes from a C version of the Fortran FFTPack library available on http://www.netlib.org/fftpack.

- int pnl\_fft\_inplace (PnlVectComplex \*data)

  Description Compute the FFT of data in place. The original content of data is lost.
- int pnl\_ifft\_inplace (PnlVectComplex \*data)

  Description Compute the inverse FFT of data in place. The original content of data is lost.
- int pnl\_fft (const PnlVectComplex \*in, PnlVectComplex \*out)

  Description Compute the FFT of in and stores it into out.
- int pnl\_ifft (const PnlVectComplex \*in, PnlVectComplex \*out)

  Description Compute the inverse FFT of in and stores it into out.
- int pnl\_fft2 (double \*re, double \*im, int n)

  Description Compute the FFT of the vector of length n whose real (resp. imaginary)

  parts are given by the arrays re (resp. im). The real and imaginary parts of the FFT are respectively stored in re and im on output.
- int pnl\_ifft2 (double \*re, double \*im, int n)

  Description Compute the inverse FFT of the vector of length n whose real (resp. imaginary) parts are given by the arrays re (resp. im). The real and imaginary parts of the inverse FFT are respectively stored in re and im on output.
- int pnl\_real\_fft (const PnlVect \*in, PnlVectComplex \*out)

  Description Compute the FFT of the real valued sequence in and stores it into out.
- int pnl\_real\_ifft (const PnlVect \*in, PnlVectComplex \*out)

  Description Compute the inverse FFT of in and stores it into out.
- int pnl\_real\_fft\_inplace (double \*data, int n)

  Description Compute the FFT of the real valued vector data of length n. The result is stored in data using the FFTPack storage described above, see 9.1.
- int pnl\_real\_ifft\_inplace (double \*data, int n)

  Description Compute the inverse FFT of the vector data of length n. data is supposed to be the FFT coefficients a real valued sequence stored using the FFTPack storage. On output, data contains the inverse FFT.
- int pnl\_real\_fft2 (double \*re, double \*im, int n)

  Description Compute the FFT of the real vector re of length n. im is only used on output to store the imaginary part the FFT. The real part is stored into re
- int pnl\_real\_ifft2 (double \*re, double \*im, int n)

  Description Compute the inverse FFT of the vector re + i \* im of length n, which is supposed to be the FFT of a real valued sequence. On exit, im is unused.

- int pnl\_fft2d\_inplace (PnlMatComplex \*data)

  Description Compute the 2D FFT of data. This function applies a 1D FFT to each row of the matrix and then a 1D FFT to each column of the modified matrix.
- int pnl\_ifft2d\_inplace (PnlMatComplex \*data)

  Description Compute the inverse 2D FFT of data. This function is the inverse of the function pnl\_fft\_2d\_inplace.
- int pnl\_fft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the 2D FFT of in and stores it into out.
- int pnl\_ifft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the inverse 2D FFT of in and stores it into out.
- int pnl\_real\_fft2d (const PnlMat \*in, PnlMatComplex \*out)

  Description Compute the 2D FFT of the real matrix in and stores it into out.
- int pnl\_real\_ifft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the inverse 2D FFT of the complex matrix in which is known to be the forward 2D FFT a real matrix. The result id stored it into out. Note that this function modifies the input matrix in.

# 10 Inverse Laplace Transform

For a real valued function f such that  $t \mapsto f(t) e^{-\sigma_c t}$  is integrable over  $\mathbb{R}^+$ , we can define its Laplace transform

$$\hat{f}(\lambda) = \int_0^\infty f(t) e^{-\lambda t} dt$$
 for  $\lambda \in \mathbb{C}$  with  $\operatorname{Re}(\lambda) \ge \sigma_c$ .

To use the following functions, you should include pnl/pnl\_laplace.h.

```
typedef struct
{
  dcomplex (*function) (dcomplex x, void *params);
  void *params;
} PnlCmplxFunc;
```

- double pnl\_ilap\_euler (PnlCmplxFunc \*fhat, double t, int N, int M)

  Description Compute f(t) where f is given by its Laplace transform fhat by numerically inverting the Laplace transform using Euler's summation. The values N = M = 15 usually give a very good accuracy. For more details on the accuracy of the method.
- double pnl\_ilap\_cdf\_euler (PnlCmplxFunc \*fhat, double t, double h, int N, int M)
   Description Compute the cumulative distribution function F(t) where F(x) = \int\_0^x f(t) dt
   and f is a density function with values on the positive real linegiven by its Laplace
   transform fhat. The computation is carried out by numerical inversion of the Laplace
   transform using Euler's summation. The values N = M = 15 usually give a very good
   accuracy. The parameter h is the discretization step, the algorithm is very sensitive to
   the choice of h.

- double  $pnl_ilap_fft$  (PnlVect \*res, PnlCmplxFunc \*fhat, double T, double eps) Description Compute f(t) for  $t \in [h, T]$  on a regular grid and stores the values in res, where h = T/size(res). The function f is defined by its Laplace transform fhat, which is numerically inverted using a Fast Fourier Transform algorithm. The size of res is related to the choice of the relative precision eps required on the value of f(t) for all  $t \leq T$ .
- double **pnl\_ilap\_gs** (**PnlFunc** \*fhat, double t, int n)

  Description Compute f(t) where f is given by its Laplace transform **fhat** by numerically inverting the Laplace transform using a weighted combination of different Gaver Stehfest's algorithms. Note that this function does not need the complex valued Laplace transform but only the real valued one. **n** is the number of terms used in the weighted combination.
- double pnl\_ilap\_gs\_basic (PnlFunc \*fhat, double t, int n)
   Description Compute f(t) where f is given by its Laplace transform fhat by numerically inverting the Laplace transform using Gaver Stehfest's method. Note that this function does not need the complex valued Laplace transform but only the real valued one. n is the number of iterations of the algorithm. Note: This function is provided for test purposes only. The function pnl\_ilap\_gs gives far more accurate results.

# 11 Ordinary differential equations

#### 11.1 Overview

To use these functionalities, you should include pnl/pnl\_integration.h.

These functions are designed for numerically solving an dimensional first of

These functions are designed for numerically solving n-dimensional first order ordinary differential equation of the general form

$$\frac{dy_i}{dt}(t) = f_i(t, y_1(t), \cdots, y_n(t))$$

The system of equations is defined by the following structure

```
typedef struct
{
  void (*function) (int neqn, double t, const double *y, double *yp, void *params);
  int neqn;
  void *params;
} PnlODEFunc;
```

- int **neqn**Description Number of equations
- void \* params
   Description An untyped structure used to pass extra arguments to the function f defining the system
- void (\* function) (int neqn, double t, const double \*y, double \*yp, void \*params)
   Description After calling the fuction, yp should be defined as follows yp\_i = f\_i(neqn, t, y, params). y and yp should be both of size neqn

We provide the following macro to evaluate a PnlODEFunc at a given point

```
#define PNL_EVAL_ODEFUNC(F, t, y, yp) \
         (*((F)->function))((F)->neqn, t, y, yp, (F)->params)
```

#### 11.2 Functions

- int pnl\_ode\_rkf45 (PnlODEFunc \*f, double \*y, double t, double t\_out, double relerr, double abserr, int \*flag)

  Description This function computes the solution of the system defined by the PnlODEFunc f at the point t\_out. On input, (t,y) should be the initial condition, abserr,relerr are the maximum absolute and relative errors for local error tests (at each step, abs(local error) should be less that relerr \* abs(y) + abserr). Note that if abserr = 0 or relerr = 0 on input, an optimal value for these variables is computed inside the function The function returns an error OK or FAIL. In case of an OK code, the y contains the solution computed at t\_out, in case of a FAIL code, flag should be examined to determine the reason of the error. Here are the different possible values for flag
  - flag = 2 : integration reached t\_out, it indicates successful return and is the normal mode for continuing integration.
  - flag = 3: integration was not completed because relative error tolerance was too small. relerr has been increased appropriately for continuing.
  - flag = 4: integration was not completed because more than 3000 derivative evaluations were needed. this is approximately 500 steps.
  - flag = 5: integration was not completed because solution vanished making a pure relative error test impossible. must use non-zero abserr to continue. using the one-step integration mode for one step is a good way to proceed.
  - flag = 6: integration was not completed because requested accuracy could not be achieved using smallest allowable stepsize. user must increase the error tolerance before continued integration can be attempted.
  - flag = 7: it is likely that rkf45 is inefficient for solving this problem. too much output is restricting the natural stepsize choice. use the one-step integrator mode. see pnl ode rkf45 step.
  - flag = 8: invalid input parameters this indicator occurs if any of the following is satisfied - neqn <= 0, t=tout, reler or abserr <= 0.</p>
- int pnl\_ode\_rkf45\_step (PnlODEFunc \*f, double \*y, double \*t, double t\_out, double \*relerr, double abserr, double \*work, int \*iwork, int \*flag)

  Description Same as pnl\_ode\_rkf45 but it only computes one step of integration in the direction of t\_out. work and iwork are working arrays of size 3 + 6 \* neqn and 5 respectively and should remain untouched between successive calls to the function. On output t holds the point at which integration stopped and y the value of the solution at that point.

# 12 Nonlinear Constrained Optimization

#### 12.1 Overview

A standard Constrained Nonlinear Optimization problem can be written as:

(O) 
$$\begin{cases} \min f(x) \\ c^{I}(x) \ge 0 \\ c^{E}(x) = 0 \end{cases}$$

where the function  $f: \mathbb{R}^n \to \mathbb{R}$  is the objective function,  $c^I: \mathbb{R}^n \to \mathbb{R}^{m_I}$  are the inequality constraints and  $c^E: \mathbb{R}^n \to \mathbb{R}^{m_E}$  are the equality constraints. These functions are supposed to be smooth.

In general, the inequality constraints are of the form  $c^{I}(x) = (g(x), x - l, u - x)$ . The vector l and u are the lower and upper bounds on the variables x and g(x) and the non linear inequality constraints.

Under some conditions, if  $x \in \mathbb{R}^n$  is a solution of problem (O), then there exist a vector  $\lambda = (\lambda^I, \lambda^E) \in \mathbb{R}^{m_I} \times \mathbb{R}^{m_E}$ , such that the well known Karush-Kuhn-Tucker (KKT) optimality conditions are satisfied:

$$(P) \begin{cases} \nabla \ell(x, \lambda^I, \lambda^E) = \nabla f(x) - \nabla c^I(x) \lambda^I - \nabla c^E(x) \lambda^E = 0 \\ c^E(x) = 0 \\ c^I(x) \ge 0 \\ \lambda^I \ge 0 \\ c^I_i(x) \lambda^I_i = 0, \ i = 1...m_I \end{cases}$$

l is known as the lagrangian of the problem (O),  $\lambda^I$  and  $\lambda^E$  as the dual variables while x is the primal variable.

#### 12.2 Functions

To use the following functions, you should include pnl/pnl\_optim.h.

To solve an inequality constrained optimization problem, ie  $m_E = 0$ , we provide the following function.

• int pnl\_optim\_intpoints\_bfgs\_solve (PnlRnFuncR\*func, PnlRnFuncRm\*grad\_func, PnlRnFuncRm\*nl\_constraints, PnlVect\*lower\_bounds, PnlVect\*upper\_bounds, PnlVect\*x\_input, double tolerance, int iter\_max, int print\_inner\_steps, PnlVect\*output)

Description This function has the following arguments:

- func is the function to minimize f.
- grad is the gradient of f. If this gradient is not available, then enter grad=NULL. In this case, finite difference will be used to estimate the gradient.
- nl\_constraints is the function q(x), ie the non linear inequality constraints.
- lower\_bounds are the lower bounds on x. Can be NULL if there is no lower bound.
- upper\_bounds are the upper bounds on x. Can be NULL if there is no upper bound.

- x\_input is the initial point where the algorithm starts.
- tolerance is the precision required in solving (P).
- iter\_max is the maximum number of iterations in the algorithm.
- print\_algo\_steps is a flag to decide to print information.
- $x_{\text{output}}$  is the point where the algorithm stops.

The algorithm returns an int, its value depends on the output status of the algorithm. We have 4 cases:

- 0: Failure: Initial point is not strictly feasible.
- 1: Step too small, we stop the algorithm.
- 2: Maximum iteration reached.
- 3: A solution has been found up to the required accuracy.

The last case is equivalent to the two inequalities:

$$||\nabla \ell(x,\lambda^I)||_{\infty} = ||\nabla f(x) - \nabla c^I(x)\lambda^I||_{\infty} < \texttt{tolerance}$$
 
$$||c^I(x)\lambda^I||_{\infty} < \texttt{tolerance}$$

where  $c^{I}(x)\lambda^{I}$  is a vector of term by term multiplication of  $c^{I}(x)$  and  $\lambda^{I}$ .

The first inequality is known as the optimality condition, the second one as the complementarity condition.

**Important Remark 1**: The algorithm we implement requires that the initial point  $x_0$ , given as an input to the algorithm, to be strictly feasible, ie:  $c(x_0) > 0$ .

**Important Remark 2**: The algorithm try to find a pair  $(x, \lambda)$  that solves the equations (P), but this does not guarantee that x is a global minimum of f on the set  $\{c(x) \ge 0\}$ .

# 13 Root finding

#### 13.1 Overview

To provide a uniformed framework to root finding functions, we use several structures for storing different kind of functions. The pointer params is used to store the extra parameters. These new types come with dedicated macros starting in PNL\_EVAL to evaluate the function and their Jacobian.

```
/*
 * f: R --> R
 * The function pointer returns f(x)
 *
typedef struct {
  double (*function) (double x, void *params);
  void *params;
} PnlFunc ;
#define PNL_EVAL_FUNC(F, x) (*((F)->function))(x, (F)->params)
```

```
/*
 * f: R^2 --> R
 * The function pointer returns f(x)
typedef struct {
  double (*function) (double x, double y, void *params);
  void *params;
} PnlFunc2D ;
#define PNL_EVAL_FUNC2D(F, x, y) (*((F)->function))(x, y, (F)->params)
/*
 * f: R --> R
 * The function pointer computes f(x) and Df(x) and stores them in fx
 * and dfx respectively
typedef struct {
  void (*function) (double x, double *fx, double *dfx, void *params);
  void *params;
} PnlFuncDFunc ;
#define PNL_EVAL_FUNC_DFUNC(F, x, fx, dfx) (*((F)->function))(x, fx, dfx, (F)->params)
/*
 * f: R^n --> R
 * The function pointer returns f(x)
typedef struct {
  double (*function) (const PnlVect *x, void *params);
  void *params;
} PnlRnFuncR ;
#define PNL_EVAL_RNFUNCR(F, x) (*((F)->function))(x, (F)->params)
/*
 * f: R^n --> R^m
 * The function pointer computes the vector f(x) and stores it in
 * fx (vector of size m)
typedef struct {
  void (*function) (const PnlVect *x, PnlVect *fx, void *params);
  void *params;
} PnlRnFuncRm ;
#define PNL_EVAL_RNFUNCRM(F, x, fx) (*((F)->function))(x, fx, (F)->params)
 * Synonymous of PnlRnFuncRm for f:R^n --> R^n
```

```
typedef PnlRnFuncRm PnlRnFuncRn;
#define PNL_EVAL_RNFUNCRN PNL_EVAL_RNFUNCRM
 * f: R^n --> R^m
* The function pointer computes the vector f(x) and stores it in fx
 * (vector of size m)
 * The Dfunction pointer computes the matrix Df(x) and stores it in dfx
 * (matrix of size m x n)
typedef struct {
 void (*function) (const PnlVect *x, PnlVect *fx, void *params);
 void (*Dfunction) (const PnlVect *x, PnlMat *dfx, void *params);
 void *params;
} PnlRnFuncRmDFunc ;
#define PNL_EVAL_RNFUNCRM_DFUNC(F, x, dfx) (*((F)->Dfunction))(x, dfx, (F)->params)
/*
 * Synonymous of PnlRnFuncRmDFunc for f:R^n --> R^m
typedef PnlRnFuncRmDFunc PnlRnFuncRnDFunc;
#define PNL_EVAL_RNFUNCRN_DFUNC PNL_EVAL_RNFUNCRM_DFUNC
```

#### 13.2 Functions

To use the following functions, you should include pnl/pnl\_root.h. For finding the zero of a real valued function we provide the following functions.

- double pnl\_root\_brent (PnlFunc\*F, double x1, double x2, double \*tol)

  Description Find the root of F between x1 and x2 with an accuracy of order tol. On exit tol is an upper bound of the error.
- int pnl\_find\_root (PnlFuncDFunc\*Func, double x\_min, double x\_max, double tol, int N\_Max, double\*res)

  Description Find the root of F between x1 and x2 with an accuracy of order tol and a maximum of N\_max iterations. On exit, the root is stored in res. Note that the function F must also compute the first derivative of the function.
- int pnl\_root\_newton (PnlFuncDFunc \*Func, double x0, double epsrel, double epsabs, int N\_max, double \*res)

  Description Find the root of F starting from x0 with an accuracy given both by epsrel and epsabs and a maximum number of iterations N\_max. On exit, the root is stored in res.Note that the function F must also compute the first derivative of the function.
- int pnl\_root\_bisection (PnlFunc \*Func, double xmin, double xmax, double epsrel, double espabs, int N\_max, double \*res)

  Description Find the root of F between x1 and x2 with an accuracy given both by epsrel and epsabs and a maximum number of iterations N\_max. On exit, the root is stored in res

Searching for the zero of a multivariate and vector valued function is a complicated problem and we rely on minpack for doing this. Here, we provide two wrappers for calling minpack routines.

- int pnl\_root\_fsolve (PnlRnFuncRnDFunc \*f, PnlVect \*x, PnlVect \*fx, double xtol, int maxfev, int \*nfev, PnlVect \*scale, int error\_msg)
   Description Compute the root of a function f: R<sup>n</sup> \( \operatorup \mathbb{R}^n \). Note that the number of components of f must be equal to the number of variates of f. This function returns OK or FAIL if something went wrong.
   Parameters
  - f is a pointer to a PnlRnFuncRnDFunc used to store the function whose root is to be found. f can also store the Jacobian of the function, if not it is computed using finite differences (see the file examples/minpack\_test.c for a usage example),
  - x contains on input the starting point of the search and an approximation of the root of f on output,
  - xtol is the precision required on x, if set to 0 a default value is used.
  - maxfev is the maximum number of evaluations of the function f before the algorithm returns, if set to 0, a coherent number is determined internally.
  - nfev contains on output the number of evaluations of f during the algorithm,
  - scale is a vector used to rescale x in a way that each coordinate of the solution is approximately of order 1 after rescaling. If on input scale=NULL, a scaling vector is computed internally by the algorithm.
  - error\_msg is a boolean (TRUE or FALSE) to specify if an error message should be printed when the algorithm stops before having converged.
  - On output, fx contains f(x).
- int pnl\_root\_fsolve\_lsq (PnlRnFuncRmDFunc \*f, PnlVect \*x, int m, PnlVect \*fx, double xtol, double ftol, double gtol, int maxfev, int \*nfev, PnlVect \*scale, int error\_-msg)

Description Compute the root of  $x \in \mathbb{R}^n \longmapsto \sum_{i=1}^m f_i(x)^2$ , note that there is no reason why m should be equal to n.

#### Parameters

- f is a pointer to a PnlRnFuncRmDFunc used to store the function whose root is to be found. f can also store the Jacobian of the function, if not it is computed using finite differences (see the file examples/minpack\_test.c for a usage example),
- x contains on input the starting point of the search and an approximation of the root of f on output,
- m is the number of components of f,
- xtol is the precision required on x, if set to 0 a default value is used.
- ftol is the precision required on f, if set to 0 a default value is used.
- gtol is the precision required on the Jacobian of f, if set to 0 a default value is used.

- maxfev is the maximum number of evaluations of the function f before the algorithm returns, if set to 0, a coherent number is determined internally.
- nfev contains on output the number of evaluations of f during the algorithm,
- scale is a vector used to rescale x in a way that each coordinate of the solution is approximately of order 1 after rescaling. If on input scale=NULL, a scaling vector is computed internally by the algorithm.
- error\_msg is a boolean (TRUE or FALSE) to specify if an error message should be printed when the algorithm stops before having converged.
- On output, fx contains f(x).

# 14 Special functions

The special function approximations are defined in the header pnl/pnl\_specfun.h.

Most of these functions rely on the *Cephes* library which uses its own error mechanism which can be activated or deactivated using the two following functions

- void **pnl\_deactivate\_mtherr** ()

  Description Deactivate Cephes error mechanism
- void **pnl\_activate\_mtherr** ()

  Description Activate Cephes error mechanism

## 14.1 Real Bessel functions

- double **pnl\_bessel\_i** (double v, double x)

  Description Modified Bessel function of the first kind of order v.
- double **pnl\_bessel\_i\_scaled** (double v, double x)

  Description Modified Bessel function of the first kind of order v divided by  $e^{|x|}$ .
- double **pnl\_bessel\_rati** (double v, double x)

  Description Ratio of modified Bessel functions of the first kind :  $I_{v+1}(x)/I_v(x)$ .
- double pnl\_bessel\_j (double v, double x)
   Description Bessel function of the first kind of order v.
- double pnl\_bessel\_j\_scaled (double v, double x)
   Description Bessel function of the first kind of order v. Same function as pnl\_bessel\_j.
- double pnl\_bessel\_y (double v, double x)
   Description Modified Bessel function of the second kind of order v.
- double pnl\_bessel\_y\_scaled (double v, double x)
   Description Modified Bessel function of the second kind of order v. Same function as pnl\_bessel\_y.
- double pnl\_bessel\_k (double v, double x)
   Description Bessel function of the third kind of order v.

- double  $pnl\_bessel\_k\_scaled$  (double v, double x)

  Description Bessel function of the third kind of order v multiplied by  $e^x$ .
- dcomplex **pnl\_bessel\_h1** (double v, double x)

  Description Hankel function of the first kind of order v.
- dcomplex pnl\_bessel\_h1\_scaled (double v, double x)

  Description Hankel function of the first kind of order v and divided by  $e^{Ix}$ .
- dcomplex pnl\_bessel\_h2 (double v, double x)
   Description Hankel function of the second kind of order v.
- dcomplex pnl\_bessel\_h2\_scaled (double v, double x)

  Description Hankel function of the second kind of order v and multiplied by  $e^{Ix}$ .

## 14.2 Complex Bessel functions

- dcomplex pnl\_complex\_bessel\_i (double v, dcomplex z)

  Description Complex Modified Bessel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_i\_scaled (double v, dcomplex z) Description Complex Modified Bessel function of the first kind of order v divided by  $e^{|Creal(z)|}$ .
- dcomplex pnl\_complex\_bessel\_rati (double v, dcomplex x) Description Ratio of complex modified Bessel functions of the first kind :  $I_{v+1}(x)/I_v(x)$ .
- dcomplex **pnl\_complex\_bessel\_j** (double v, dcomplex z)

  Description Complex Bessel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_j\_scaled (double v, dcomplex z)

  Description Complex Bessel function of the first kind of order v divided by  $e^{|Cimag(z)|}$ .
- dcomplex pnl\_complex\_bessel\_y (double v, dcomplex z)

  Description Complex Modified Bessel function of the second kind of order v.
- dcomplex pnl\_complex\_bessel\_y\_scaled (double v, dcomplex z) Description Complex Modified Bessel function of the second kind of order v divided by  $_{\rho}|Cimag(z)|$
- dcomplex pnl\_complex\_bessel\_k (double v, dcomplex z)
   Description Complex Bessel function of the third kind of order v.
- dcomplex pnl\_complex\_bessel\_k\_scaled (double v, dcomplex z) Description Complex Bessel function of the third kind of order v multiplied by  $e^z$ .
- dcomplex **pnl\_complex\_bessel\_h1** (double v, dcomplex z)

  Description Complex Hankel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_h1\_scaled (double v, dcomplex z)

  Description Complex Hankel function of the first kind of order v and divided by  $e^{Iz}$ .

- dcomplex pnl\_complex\_bessel\_h2 (double v, dcomplex z)

  Description Complex Hankel function of the second kind of order v.
- dcomplex pnl\_complex\_bessel\_h2\_scaled (double v, dcomplex z) Description Complex Hankel function of the second kind of order v and multiplied by  $e^{Iz}$ .

#### 14.3 Error functions

- double **pnl\_sf\_erf** (double x) Description Compute  $\frac{2}{\pi} \int_0^\infty e^{-t^2} dt$
- double **pnl\_sf\_erfc** (double x) Description Compute  $1. - \frac{2}{\pi} \int_0^\infty e^{-t^2} dt$
- double **pnl\_sf\_log\_erf** (double x)

  Description Compute log pnl\_sf\_erf(x)
- double **pnl\_sf\_log\_erfc** (double x)

  Description Compute log pnl\_sf\_erfc(x)

#### 14.4 Gamma functions

For x > 0, the Gamma Function is defined by

$$\Gamma(x) = \int_0^\infty e^{-u} u^{x-1} du.$$

- double  $pnl\_sf\_fact$  (int n) Description Computes factorial of  $n \Gamma(n+1)$ .
- double **pnl\_sf\_gamma** (double x) Description Computes  $\Gamma(x), x \geq 0$
- double pnl\_sf\_log\_gamma (double x) Description Computes  $\log(\Gamma(x)), x \geq 0$
- int pnl\_sf\_log\_gamma\_sgn (double x, double \*y, int \*sgn)

  Description Computes  $y = \log(|\Gamma(x)|)$  for x > 0 sgn contains the sign of  $\Gamma(x)$  (-1 or +1).
- double pnl\_sf\_choose (int n, int k)

  Description Computes the binomial coefficient  $\binom{n}{k} = \frac{n!}{k!(n-k)!}$  for  $0 \le k \le n$  in double precision.

## 14.5 Digamma function

For x > 0, the digamma function  $\psi$  is defined as the logarithmic derivative of the Gamma function  $\Gamma$ 

$$\psi(x) = \frac{d}{dx} \log \Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}.$$

The function  $\psi$  admits the following integral representation

$$\psi(x) = \int_0^\infty \left( \frac{e^{-u}}{u} - \frac{e^{-xu}}{1 - e^{-u}} \right).$$

#### 14.6 Incomplete Gamma functions

For  $a \in \mathbb{R}$  and x > 0, the Incomplete Gamma Function is defined by

$$\Gamma(a,x) = \int_{x}^{\infty} e^{-u} u^{a-1} du.$$

A relation similar to the one existing for the standard Gamma function holds

$$\Gamma(a,x) = \frac{-x^a e^{-x} + \Gamma(a+1,x)}{a}.$$

$$\begin{split} \Gamma(a) &= \int_0^\infty u^{a-1} \operatorname{e}^{-u} du \\ P(a,x) &= \frac{\Gamma(a) - \Gamma(a,x)}{\Gamma(a)} = \frac{1}{\Gamma(a)} \int_0^x u^{a-1} \operatorname{e}^{-u} du \\ Q(a,x) &= 1 - P(a,x) = \frac{\Gamma(a,x)}{\Gamma(a)} = \frac{1}{\Gamma(a)} \int_x^\infty \operatorname{e}^{-u} u^{a-1} du. \end{split}$$

- double **pnl\_sf\_gamma\_inc** (double a, double x) Description Computes  $\Gamma(a, x)$ ,  $a \in \mathbb{R}, x \geq 0$
- void pnl\_sf\_gamma\_inc\_P (double a, double x) Description Computes P(a, x),  $a > 0, x \ge 0$
- void **pnl\_sf\_gamma\_inc\_Q** (double a, double x) Description Computes Q(a, x),  $a > 0, x \ge 0$

#### 14.7 Exponential integrals

For x > 0 and  $n \in \mathbb{N}$ , the function  $E_n$  is defined by

$$E_n(x) = \int_1^\infty e^{-xu} u^{-n} du$$

This function is linked to the Incomplete Gamma function by

$$E_n(x) = \int_x^\infty e^{-xu} (xu)^{-n} x^{n-1} d(xu) = x^{n-1} \int_x^\infty e^{-t} t^{-n} dt = x^{n-1} \Gamma(1-n, x),$$

from which we can deduce

$$nE_{n+1}(x) = e^{-x} - xE_n(x).$$

For n > 1, the series expansion is given by

$$E_n(x) = x^{n-1}\Gamma(1-n) + \left[ -\frac{1}{1-n} + \frac{x}{2-n} - \frac{x^2}{2(3-n)} + \frac{x^3}{6(4-n)} - \dots \right].$$

The asymptotic behaviour is given by

$$E_n(x) = \frac{e^{-x}}{x} \left[ 1 - \frac{n}{x} + \frac{n(n+1)}{x^2} + \ldots \right].$$

The special case n=1 gives

$$E_1(x) = \int_x^\infty \frac{e^{-u}}{u} du, \quad |\operatorname{Arg}(x)| \ge \pi.$$

For any complex number x with positive real part, this can be written

$$E_1(x) = \int_1^\infty \frac{e^{-ux}}{u} du, \quad \Re(x) \ge 0.$$

By integrating the Taylor expansion of  $e^{-t}/t$ , and extracting the logarithmic singularity, we can derive the following series representation for  $E_1(x)$ ,

$$E_1(x) = -\gamma - \ln x - \sum_{k=1}^{\infty} \frac{(-1)^k x^k}{k \, k!} \qquad |\text{Arg}(x)| < \pi.$$

The function  $E_1$  is linked to the exponential integral Ei

$$Ei(x) = \int_{-\infty}^{x} \frac{e^{u}}{u} du = -\int_{-x}^{\infty} \frac{e^{-u}}{u} du \quad \forall x \neq 0.$$

The above definition can be used for positive values of x, but the integral has to be understood in terms of its Cauchy principal value, due to the singularity of the integrand at zero.

$$Ei(-x) = -E_1(x), \quad \Re(x) > 0.$$

We deduce,

$$Ei(x) = \gamma + \ln x + \sum_{k=1}^{\infty} \frac{x^k}{k \, k!}, \quad x > 0.$$

For  $x \in \mathbb{R}$ 

$$\Gamma(0,x) = \begin{cases} -Ei(-x) - i\pi & x < 0, \\ -Ei(-x) & x > 0. \end{cases}$$

• double **pnl\_sf\_expint\_En** (int n, double x) Description Computes  $E_n(x)$  for  $n \ge 0, x \ge 0$ , or x > 0 when n = 0 or 1.

#### 14.8 Hypergeometric functions

- double pnl\_sf\_hyperg\_2F1 (double a, double b, double c, double x)
   Description Compute the Gauss hypergeometric function 2F1(a,b,c,x) for |x| < 1 and for x < -1 when b,a,c,(b-a),(c-a),(c-b) are not integers</li>
- double pnl\_sf\_hyperg\_1F1 (double a, double b, double x)
   Description Compute the hypergeometric function 1F1(a,b,x)

- double pnl\_sf\_hyperg\_2F0 (double a, double b, double x)

  Description Compute the hypergeometric function 2F0(a,b,x) for x<0 using the relation  $2F0(a,b,x) = (-x)^{-a}U(a,1+a-b,-\frac{1}{x}).$
- double pnl\_sf\_hyperg\_0F1 (double c, double x)
   Description Compute the hypergeometric function 0F1(c,x)
- double pnl\_sf\_hyperg\_U (double a, double b, double x)
   Description Compute the confluent hypergeometric function U(a,b,x) with x > 0

# 15 Some bindings

#### 15.1 MPI bindings

#### 15.1.1 Overview

We provide some bindings for the MPI library to natively handle *PnlObjects*. The functionnalities described in this chapter are declared in pnl/pnl\_mpi.h.

#### 15.1.2 Functions

All the following functions return an error code as an integer value. This returned value should be tested against MPI\_SUCCESS to check that no error occurred.

- int pnl\_object\_mpi\_pack\_size (const PnlObject \*Obj, MPI\_Comm comm, int \*size)
  - Description Compute in size the amount of space needed to pack Obj.
- int pnl\_object\_mpi\_pack (const PnlObject \*Obj, void \*buf, int bufsize, int \*pos, MPI\_Comm comm)

  Description Pack Obj into buf which must be at least of length size. size must be at least equal to the value returned by pnl object mpi pack size.
- int pnl\_object\_mpi\_unpack (PnlObject \*Obj, void \*buf, int bufsize, int \*pos, MPI\_Comm comm)

  Description Unpack the content of buf starting at position pos (unless several objects have been packed contiguously, \*pos should be equal to 0). buf is a contiguous memery area of length bufsize (note that the size is counted in bytes). pos is incremented and is on output the first location in the input buffer after the locations occupied by the message that was unpacked. pos is properly set for a future call to MPI\_Unpack if any.
- int pnl\_object\_mpi\_send (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm)

  Description Perform a standard-mode blocking send of Obj. The object is sent to the process with rank dest.
- int pnl\_object\_mpi\_ssend (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm)

  Description Perform a standard-mode synchronous blocking send of Obj. The object is sent to the process with rank dest.

- int pnl\_object\_mpi\_recv (PnlObject \*Obj, int src, int tag, MPI\_Comm comm, MPI\_Status \*status)

  Description Perform a standard-mode blocking receive of Obj. The object is sent to the process with rank dest. Note that Obj should be an already allocated object and that its type should match the true type of the object to be received. src is the rank of the process who sent the object.
- int pnl\_object\_mpi\_bcast (PnlObject \*Obj, int root, MPI\_Comm comm)

  Description Broadcast the object Obj from the process with rank root to all other processes of the group comm.
- int pnl\_object\_mpi\_reduce (PnlObject \*Recvbuf, const PnlObject \*Sendbuf, MPI\_Op op, int root, MPI\_Comm comm)

  Description Perform the reduction described by op on the objects Sendbuf and stores the result into Recvbuf. Note that Recvbuf and Sendbuf must be of the same type. The argument root is the index of the root process and comm is a communicator. Not all reductions are implemented for all types. Here is the list of compatible reductions

$MPI\_SUM$	PnlVect, PnlVectInt, PnlVectComplex,
	PnlMat, PnlMatInt, PnlMatComplex
MPI_PROD, MPI_MAX,	PnlVect, PnlVectInt, PnlMat, PnlMatInt
MPI MIN	

For more expect users, we provide the following nonblocking functions.

- int pnl\_object\_mpi\_isend (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm, MPI\_Request \*request)

  Description Start a standard-mode, nonblocking send of object Obj to the process with rank dest.
- int pnl\_object\_mpi\_irecv (void \*\*buf, int \*size, int src, int tag, MPI\_Comm comm, int \*flag, MPI\_Request \*request)

  Description Start a standard-mode, nonblocking receive of object Obj from the process with rank root. On output flag equals to TRUE if the object can be received and FALSE otherwise (this is the same as for MPI\_Iprobe).

#### 15.2 The save/load interface

The interface is only accessible when the MPI bindings are compiled since it is based on the Packing/Unpacking facilities of MPI.

The functionnalities described in this chapter are declared in pnl/pnl\_mpi.h.

- PnlRng\*\* pnl\_rng\_create\_from\_file (char \*str, int n)

  Description Load n rng from the file of name str and returns an array of n PnlRng.
- int pnl\_rng\_save\_to\_file (PnlRng \*\*rngtab, int n, char \*str)

  Description Save n rng stored in rngtab into the file of name str.

- int pnl\_object\_save (PnlObject \*O, FILE \*stream)

  Description Save the object 0 into the stream stream. stream is typically created by calling fopen with mode="wb". This function can be called several times to save several objects in the same stream.
- PnlObject\* pnl\_object\_load (FILE \*stream)
   Description Load an object from the stream stream. stream is typically created by calling fopen with mode="rb". This function can be called several times to load several objects from the same stream. If stream was empty or it did not contain any PnlObjects, the function returns NULL.
- PnlList\* pnl\_object\_load\_into\_list (FILE \*stream)

  Description Load as many objects as possible from the stream stream and stores them into a PnlList. stream is typically created by calling fopen with mode="rb". If stream was empty or it did not contain any PnlObjects, the function returns NULL.

# 16 Financial functions

The financial functions are defined in the header pnl/pnl\_finance.h.

- int pnl\_cf\_call\_bs (double s, double k, double T, double r, double divid, double sigma, double \*ptprice, double \*ptdelta)

  Description Compute the price and delta of a call option (s k)\_+ in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid. The parameters ptprice and ptdelta are respectively set to the price and delta on output.
- int pnl\_cf\_put\_bs (double s, double k, double T, double r, double divid, double sigma, double \*ptprice, double \*ptdelta)
   Description Compute the price and delta of a put option (k s)+ in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid. The parameters ptprice and ptdelta are respectively set to the price and delta on output.
- double pnl\_bs\_call (double s, double k, double T, double r, double divid, double sigma)
   Description Compute the price of a call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double pnl\_bs\_put (double s, double k, double T, double r, double divid, double sigma)
   Description Compute the price a put option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double **pnl\_bs\_call\_put** (int iscall, double s, double k, double T, double r, double divid, double sigma)

Description Compute the price of a put option if iscall=0 or a call option if iscall=1 with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.

double pnl\_bs\_vega (double s, double k, double T, double r, double divid, double sigma)
 Description Compute the vega of a put or call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and

dividend rate divid.

double pnl\_bs\_gamma (double s, double k, double T, double r, double divid, double sigma)
 Description Compute the gamma of a put or call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.

Practitioners do not speak in terms of option prices, but rather compare prices in terms of their implied Black & Scholes volatilities. So this parameter is very useful in practice. Here, we propose two functions to compute  $\sigma_{impl}$ : the first one is for one up-let, maturity, strike, option price. the second function is for a list of strikes and maturities, a matrix of prices (with strikes varying row-wise).

- double pnl\_bs\_implicit\_vol (int is\_call, double Price, double s, double K, double T, double r, double divid, int \*error)

  Description Compute the implied volatility of a put option if iscall=0 or a call option if iscall=1 with spot s and strike K in the Black-Scholes model with instantaneous interest rate r, maturity T and dividend rate divid. On output error is OK if the computation of the implied volatility succeeded or FAIL if it failed.
- int pnl\_bs\_matrix\_implicit\_vol (const PnlMatInt \*iscall, const PnlMat \*Price, double s, double r, double divid, const PnlVect \*K, const PnlVect \*T, PnlMat \*Vol)

  Description Compute the matrix of implied volatilities Vol(i,j) of a put option if iscall(i,j)=0 or a call option if iscall(i,j)=1 with spot s and strike K(j) in the Black-Scholes model with instantaneous interest rate r, maturity T(j) and dividend rate divid. This function returns the number of failures, when everything succeeded it returns 0.

# Index

A	Creal
ABS	CRmul
ADS12	CRsub
C	Crisub
C op amcb	Csinh
C_op_amib	Csqr norm
C_op_apcb	<u>. —</u>
C_op_apib	Csqrt
C op damb	Csub
C_op_damb	
C_op_damib	Ctanh
	Ctgamma
C_op_dapb	CUB
C_op_dapcb	CZERO
C_op_dapib	D
C_op_idamb	DBL EPSILON11
C_op_idamcb	DBL MAX
C_op_idapb	DOUBLE_MAX
C_op_idapcb	DOUBLE_MAX11
Cabs	G
Cadd	GET
Carg	GET IMAG
Ccos	GET_REAL
Ccosh	GET_IEME20
Ccotan	I
Ccotanh	INT MAX11
Cdiv14	_
Cexp	L
CI13	LET20
CIexp	LET_IMAG25
Cimag	LET_REAL
Cinv14	
Clgamma	M
Clog14	M_1_PI11
Cminus	M_1_SQRT2PI11
Cmul	M_2_PI11
Complex14	M_2_SQRTPI11
Complex_polar14	M_2PI11
CONE13	M_E11
Conj14	M_EULER11
Cpow15	M_LN1011
Cpow_real	M_LN211
Cprintf	M_LOG10E11
CRadd	M_LOG2E11
CRdiv14	M_PI11

M DI 0	1 1 1 4 : 1 45
M_PI_211	pnl_band_mat_map_inplace45
M_PI_4	pnl_band_mat_minus_band_mat 44
M_SQRT1_211	pnl_band_mat_minus_double44
M_SQRT211	pnl_band_mat_mult_band_mat_term . 45
M_SQRT2_PI11	pnl_band_mat_mult_double44
M_SQRT2PI11	pnl_band_mat_mult_vect_inplace 45
MAX11	pnl_band_mat_new
MAX_INT11	PNL_BAND_MAT_OBJECT7
MGET	pnl_band_mat_plus_band_mat44
MIN	pnl_band_mat_plus_double44
MLET30	pnl_band_mat_print_as_full44
MLE1	
N	pnl_band_mat_resize
	pnl_band_mat_set
NAN11	pnl_band_mat_set_double44
D	pnl_band_mat_syslin45
P	pnl_band_mat_syslin_inplace45
pnl_acosh	pnl_band_mat_to_mat44
pnl_activate_mtherr81	PNL_BASIS_CANONICAL63
PNL_ALTERNATE11	pnl_basis_clone
pnl_array_clone10	pnl_basis_copy
pnl_array_copy10	pnl basis create
pnl_array_create10	pnl_basis_create_from_degree64
pnl_array_free	pnl_basis_create_from_hyperbolic_degree
pnl_array_get	66
pm_anay_gco	DD
nnl array now 10	
pnl_array_new	pnl_basis_create_from_prod_degree $\dots65$
pnl_array_print10	pnl_basis_create_from_prod_degree 65 pnl_basis_create_from_tensor 65
pnl_array_print	pnl_basis_create_from_prod_degree 65 pnl_basis_create_from_tensor 65 pnl_basis_eval 68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10	pnl_basis_create_from_prod_degree 65pnl_basis_create_from_tensor 65pnl_basis_eval 68pnl_basis_eval_D 68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13	pnl_basis_create_from_prod_degree 65 pnl_basis_create_from_tensor 65 pnl_basis_eval 68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10	pnl_basis_create_from_prod_degree 65pnl_basis_create_from_tensor 65pnl_basis_eval 68pnl_basis_eval_D 68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13	pnl_basis_create_from_prod_degree65pnl_basis_create_from_tensor65pnl_basis_eval68pnl_basis_eval_D68pnl_basis_eval_D268
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13	pnl_basis_create_from_prod_degree65pnl_basis_create_from_tensor65pnl_basis_eval68pnl_basis_eval_D68pnl_basis_eval_D268pnl_basis_eval_D2_vect67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44	pnl_basis_create_from_prod_degree.65pnl_basis_create_from_tensor.65pnl_basis_eval.68pnl_basis_eval_D.68pnl_basis_eval_D2.68pnl_basis_eval_D2_vect.67pnl_basis_eval_D_vect.67pnl_basis_eval_derivs.68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43	pnl_basis_create_from_prod_degree.65pnl_basis_create_from_tensor.65pnl_basis_eval.68pnl_basis_eval_D.68pnl_basis_eval_D2.68pnl_basis_eval_D2_vect.67pnl_basis_eval_D_vect.67pnl_basis_eval_derivs.68pnl_basis_eval_derivs.68pnl_basis_eval_derivs_vect.67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43	pnl_basis_create_from_prod_degree.65pnl_basis_create_from_tensor.65pnl_basis_eval.68pnl_basis_eval_D.68pnl_basis_eval_D2.68pnl_basis_eval_D2_vect.67pnl_basis_eval_D_vect.67pnl_basis_eval_derivs.68pnl_basis_eval_derivs_vect.67pnl_basis_eval_derivs_vect.67pnl_basis_eval_vect.67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45	pnl_basis_create_from_prod_degree.65pnl_basis_create_from_tensor.65pnl_basis_eval.68pnl_basis_eval_D.68pnl_basis_eval_D2.68pnl_basis_eval_D2_vect.67pnl_basis_eval_derivs.68pnl_basis_eval_derivs.68pnl_basis_eval_derivs_vect.67pnl_basis_eval_vect.67pnl_basis_eval_seval_vect.67pnl_basis_fit_ls.66
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44	pnl_basis_create_from_prod_degree       .65         pnl_basis_create_from_tensor       .65         pnl_basis_eval       .68         pnl_basis_eval_D       .68         pnl_basis_eval_D2       .68         pnl_basis_eval_D2_vect       .67         pnl_basis_eval_derivs       .68         pnl_basis_eval_derivs       .68         pnl_basis_eval_derivs_vect       .67         pnl_basis_eval_vect       .67         pnl_basis_fit_ls       .66         pnl_basis_free       .66
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43	pnl_basis_create_from_prod_degree       65         pnl_basis_create_from_tensor       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44	pnl_basis_create_from_prod_degree       .65         pnl_basis_create_from_tensor       .65         pnl_basis_eval       .68         pnl_basis_eval_D       .68         pnl_basis_eval_D2       .68         pnl_basis_eval_D2_vect       .67         pnl_basis_eval_derivs       .68         pnl_basis_eval_derivs_vect       .67         pnl_basis_eval_vect       .67         pnl_basis_fit_ls       .66         pnl_basis_free       .66         PNL_BASIS_HERMITE       .63         pnl_basis_i       .68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45	pnl_basis_create_from_prod_degree       65         pnl_basis_create_from_tensor       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_lAxpby       45	pnl_basis_create_from_prod_degree       65         pnl_basis_create_from_tensor       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_free       43         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_lAxpby       45         pnl_band_mat_lget       44	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i_D       68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_lAxpby       45         pnl_band_mat_lget       44         pnl_band_mat_let       44         pnl_band_mat_let       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i       67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_laxpby       45         pnl_band_mat_liget       44         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i_D       68
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_lAxpby       45         pnl_band_mat_lget       44         pnl_band_mat_let       44         pnl_band_mat_let       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i       67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_create_from_mat       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_inv_term       45         pnl_band_mat_laxpby       45         pnl_band_mat_liget       44         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       67         pnl_basis_i       67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_laxpby       45         pnl_band_mat_leet       44         pnl_band_mat_leet       44         pnl_band_mat_lu       45         pnl_band_mat_lu       45         pnl_band_mat_lu_syslin_inplace       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_derivs_vect       67         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_ii       67         pnl_basis_ii       67         pnl_basis_ii       67         pnl_basis_ii       67         pnl_basis_ii       67
pnl_array_print       10         pnl_array_resize       10         pnl_array_set       10         pnl_asinh       13         pnl_atanh       13         pnl_band_mat_clone       44         pnl_band_mat_copy       44         pnl_band_mat_create       43         pnl_band_mat_div_band_mat_term       45         pnl_band_mat_div_double       44         pnl_band_mat_free       43         pnl_band_mat_get       44         pnl_band_mat_laxpby       45         pnl_band_mat_leet       44         pnl_band_mat_lu       45         pnl_band_mat_lu_syslin       46         pnl_band_mat_nat       45         pnl_band_mat_nat       45         pnl_band_mat_nat       45         pnl_band_mat_nat       45         pnl_band_mat_nat       46         pnl_band_mat_nat       45         pnl_band_mat_nat       45         pnl_band_mat_nat       45         pnl_band_mat_nat       45	pnl_basis_create_from_prod_degree       65         pnl_basis_eval       68         pnl_basis_eval_D       68         pnl_basis_eval_D2       68         pnl_basis_eval_D2_vect       67         pnl_basis_eval_D_vect       67         pnl_basis_eval_derivs       68         pnl_basis_eval_vect       67         pnl_basis_fit_ls       66         pnl_basis_free       66         PNL_BASIS_HERMITE       63         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       68         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_i       67         pnl_basis_ii, vect       67         pnl_basis_ik_vect       67

pnl_basis_print	pnl_cell_new
pnl_basis_set_domain	pnl cf call bs
pnl_basis_set_from_tensor66	pnl_cf_put_bs
pnl_basis_set_reduced66	pnl cg solver create
PNL_BASIS_TCHEBYCHEV63	pnl_cg_solver_free51
pnl_basis_type_register64	pnl_cg_solver_initialisation51
pnl_bessel_h181	pnl_cg_solver_new51
pnl_bessel_h1_scaled	pnl_cg_solver_solve
pnl_bessel_h281	pnl_complex_bessel_h182
pnl_bessel_h2_scaled	pnl_complex_bessel_h1_scaled82
pnl bessel i	pnl complex bessel h282
pnl_bessel_i_scaled81	pnl_complex_bessel_h2_scaled82
pnl_bessel_j	pnl_complex_bessel_i82
pnl bessel j scaled	pnl_complex_bessel_i_scaled82
pnl_bessel_k	pnl_complex_bessel_j
pnl_bessel_k_scaled	pnl_complex_bessel_j_scaled82
pnl bessel rati	pnl_complex_bessel_k82
pnl bessel y	pnl_complex_bessel_k_scaled 82
pnl bessel y scaled	pnl_complex_bessel_rati82
pnl_bicg_solver_create	pnl_complex_bessel_y82
pnl_bicg_solver_free51	pnl_complex_bessel_y_scaled 82
pnl_bicg_solver_initialisation51	pnl_cosm1
pnl_bicg_solver_new	pnl_dcmt_create_array63
pnl_bicg_solver_solve51	pnl_dcmt_free
pnl_bs_call	pnl_dcmt_free_array
pnl_bs_call_put	pnl_dcmt_genrand_double63
pnl_bs_gamma 88	pnl_dcmt_get_parameter63
pnl_bs_implicit_vol 89	pnl_deactivate_mtherr81
pnl_bs_matrix_implicit_vol89	pnl_expm113
pnl_bs_put	pnl_fft
pnl_bs_vega	pnl_fft271
pnl_cdf2nor	pnl_fft2d72
pnl_cdf_bet53	pnl_fft2d_inplace
pnl_cdf_bin54	pnl_fft_inplace71
pnl_cdf_chi54	pnl_find_root
pnl_cdf_chn	PNL_GET_PARENT_TYPE8
pnl_cdf_f54	PNL_GET_TYPE7
pnl_cdf_fnc54	PNL_GET_TYPENAME7
pnl_cdf_gam54	pnl_gmres_solver_create52
pnl_cdf_nbn54	pnl_gmres_solver_free52
pnl_cdf_nor54	pnl_gmres_solver_initialisation 52
pnl_cdf_poi54	pnl_gmres_solver_new52
pnl_cdf_t54	pnl_gmres_solver_solve
pnl_cdfbchi2n	pnl_hmat_clone
pnl_cdfchi2n	pnl_hmat_copy
pnl_cdfnor 55	pnl_hmat_create
pnl_cell_free9	pnl_hmat_create_from_double47

pnl_hmat_create_from_ptr47	pnl list remove i	9
pnl_hmat_free	pnl_list_remove_last	
pnl_hmat_get	pnl_log1p	13
pnl_hmat_lget	pnl_lround	
pnl_hmat_mult_double48	pnl_ltrunc	12
pnl_hmat_new	pnl_mat_axpy	
PNL_HMAT_OBJECT7	pnl_mat_bicg_solver_solve	
pnl_hmat_plus_hmat48	pnl_mat_cg_solver_solve	
pnl_hmat_print	pnl_mat_chol	
pnl_hmat_resize	pnl_mat_chol_syslin	
pnl_hmat_set	pnl_mat_chol_syslin_inplace	
pnl_ifft71	pnl_mat_chol_syslin_mat	
pnl_ifft2	pnl_mat_clone	
pnl_ifft2d	pnl_mat_col_permute	
pnl_ifft2d_inplace	pnl_mat_copy	
pnl_ifft_inplace	pnl_mat_create	
pnl_ilap_cdf_euler	pnl_mat_create_diag	
pm_nap_euler	pnl_mat_create_diag_from_ptr pnl_mat_create_from_double	
pnl_ilap_gs	pnl_mat_create_from_file	
pnl_ilap_gs_basic	pnl mat create from list	
PNL INF	pnl_mat_create_from_ptr	
pnl_integration	pnl_mat_cross	
pnl_integration_2d69	pnl_mat_cumprod	
pnl_integration_GK	pnl_mat_cumsum	
pnl_integration_GK2D69	pnl_mat_dgemm	
pnl_integration_qag69	pnl_mat_dgemv	
pnl_integration_qagp70	pnl_mat_dger	
pnl_integration_qng	pnl_mat_div_double	30
pnl_integration_qng_2d69	pnl_mat_div_mat_term	31
pnl_inv_cdfnor55	pnl_mat_eigen	37
pnl_iround	pnl_mat_eq	
PNL_IS_EVEN11	pnl_mat_eq_double	32
PNL_IS_ODD11	pnl_mat_exp	35
pnl_itrunc12	pnl_mat_extract_subblock	
pnl_lgamma12	pnl_mat_find	
pnl_list_clone9	pnl_mat_fprint	
pnl_list_concat9	pnl_mat_fprint_nsp	
pnl_list_copy	pnl_mat_free	
pnl_list_free9	pnl_mat_get	
pnl_list_get9	pnl_mat_get_col	
pnl_list_insert_first9	pnl_mat_get_row	
pnl_list_insert_last	pnl_mat_gmres_solver_solve	
pnl_list_new	pnl_mat_inverse	
PNL_LIST_OBJECT7	pnl_mat_inverse_with_chol	
pnl_list_print	pnl_mat_lAxpby	
pnl_list_remove_first9	pnl_mat_lget	29

pnl_mat_log37	pnl_mat_rng_uni	58
pnl_mat_lower_inverse	pnl_mat_rng_uni2	
pnl mat lower syslin	pnl_mat_row_permute	
pnl_mat_ls	pnl_mat_scalar_prod	
pnl_mat_ls_mat	pnl_mat_set	
pnl_mat_lu35	pnl_mat_set_col	
pnl_mat_lu_syslin	pnl_mat_set_diag	
pnl_mat_lu_syslin_inplace36	pnl_mat_set_double	
pnl_mat_lu_syslin_mat	pnl_mat_set_from_ptr	
pnl_mat_map31	pnl mat set id	
pnl_mat_map_inplace31	pnl_mat_set_row	
pnl_mat_map_mat31	pnl_mat_set_zero	
pnl_mat_map_mat_inplace	pnl_mat_sq_transpose	
pnl_mat_max32	pnl mat sum	
pnl mat max index	pnl_mat_sum_vect	
pnl_mat_min	pnl_mat_swap_rows	
pnl_mat_min_index	pnl mat syslin	
pnl mat minmax	pnl_mat_syslin_inplace	
pnl_mat_minmax		
pnl_mat_minus_double	pnl_mat_syslin_mat pnl_mat_tr	
	-	
pnl_mat_minus_mat	pnl_mat_transpose pnl_mat_upper_inverse	
-		
pnl_mat_mult_mat	pnl_mat_upper_syslin	
pnl_mat_mult_mat_inplace	pnl_mat_wrap_array	
pnl_mat_mult_mat_term	pnl_mat_wrap_hmat	
pnl_mat_mult_vect	pnl_mat_wrap_vect pnl_mt_genrand	
pnl_mat_mult_vect_transpose 34	pnl_mt_genrand_double pnl_mt_sseed	
pnl_mat_mult_vect_transpose_inplace .34 pnl mat new	PNL_NEGINF	
PNL_MAT_OBJECT	pnl_normal_density	
pnl_mat_pchol35	PNL_OBJECT	
pnl mat plus double30	pnl object create	
pnl_mat_plus_mat	pnl_object_load	
pnl mat print	pnl_object_load_into_list	
. – –		
pnl_mat_print_nsp	pnl_object_mpi_bcast pnl_object_mpi_irecv	
pnl_mat_prod_vect31	pnl_object_mpi_isend	
pnl_mat_qr37	pnl_object_mpi_pack	
pnl_mat_qr_syslin37	pnl_object_mpi_pack_size	
pnl_mat_qsort32	pnl_object_mpi_recv	
pnl_mat_qsort_index32	pnl_object_mpi_reduce	
pnl_mat_rand_normal	pnl_object_mpi_send pnl_object_mpi_ssend	
pnl_mat_rand_uni2	pnl_object_mpi_unpack	
pnl_mat_resize	pnl_object_save	
pnl_mat_rng_normal	pnl_ode_rkf45	
pm_mat_rng_normat	pm_0uc_1ki40	14

nnl ode virf45 eten 7	5 ppl mg init 57
pnl_ode_rkf45_step	1 — 9—
pnl_permutation_create3	<u> </u>
pnl permutation fprint	1 _ 0_
pnl_permutation_free	— · · · — · · · · · · · · · · · · · · ·
pnl_permutation_inverse3	r _ O_r
pnl_permutation_new	1 0_1
pnl_permutation_print3	I = 0=::::::::::::::::::::::::::::::::::
PNL POSINF 1	r 0
pnl_rand_bernoulli 6	Pm_ins_seeca
pnl_rand_bessel 6	Pm_1116_4111
pnl rand chi2 6	piiiiii8aiiiab
pnl_rand_exp6	0 pnl root brent
pnl_rand_gamma6	pm_1000_b10m0
pnl_rand_gauss6	pnl_root_fsolve_lsq80
pnl_rand_init6	0 pnl_root_newton
pnl_rand_name6	0 pnl_round
pnl_rand_normal6	0 pnl_sf_choose83
pnl_rand_or_quasi 6	0 pnl sf erf82
pnl_rand_poisson6	0 pnl sf erfc82
pnl_rand_poisson16	0 pnl_sf_expint_En85
pnl_rand_sseed	0 pnl_sf_fact83
pnl_rand_uni6	0 pnl_sf_gamma83
pnl_rand_uni_ab6	0 pnl_sr_gamma_inc
pnl_real_fft7	/.
pnl_real_fft2	pnl_sf_gamma_inc_P84
pnl_real_fft2d7	pnl_sf_gamma_inc_Q84
pnl_real_fft_inplace	pnl_sf_hyperg_0F185
pnl_real_ifft	2 pnl_sf_hyperg_1F185
pnl_real_ifft2 7	1 -f 1 0F1
pnl_real_ifft2d7	1 C 1 TT 0F
pnl_real_ifft_inplace7	
pnl_rng_bernoulli5	7 pnl_sf_log_erf83
pnl_rng_bessel5	1 6 1
pnl_rng_chi25	
pnl_rng_clone 5	DAIL GLOST
pnl_rng_copy5	1
pnl_rng_create5	
pnl_rng_create_from_file8	
pnl_rng_dcmt_create_array5	
pnl_rng_dcmt_create_array_id 5	
pnl_rng_dcmt_create_id5	
pnl_rng_exp5	
pnlrngfree	
pnl_rng_gamma5	
pnl_rng_gauss5	
pnl_rng_get_from_id5	7 pnl_tridiag_mat_div_double 41

1 1.	1 11	0.0
pnl_tridiag_mat_div_tridiag_mat_term	pnl_vect_compact_set_double	
41	pnl_vect_compact_set_ptr	
pnl_tridiag_mat_fprint41	pnl_vect_compact_to_pnl_vect	
pnl_tridiag_mat_free40	pnl_vect_complex_create_from_array .	
pnl_tridiag_mat_get40	pnl_vect_complex_get_imag	. 24
pnl_tridiag_mat_lAxpby42	pnl_vect_complex_get_real	.24
pnl_tridiag_mat_lget40	pnl_vect_complex_lget_imag	. 24
pnl_tridiag_mat_lu_clone	pnl_vect_complex_lget_real	. 24
pnl_tridiag_mat_lu_compute42	pnl_vect_complex_mult_double	. 24
pnl_tridiag_mat_lu_copy	pnl_vect_complex_set_imag	
pnl_tridiag_mat_lu_create	pnl_vect_complex_set_real	
pnl_tridiag_mat_lu_free	pnl_vect_complex_split_in_array	
pnl_tridiag_mat_lu_new	pnl_vect_complex_split_in_vect	
pnl_tridiag_mat_lu_resize42	pnl_vect_copy	
pnl_tridiag_mat_lu_syslin	pnl_vect_create	
pnl_tridiag_mat_lu_syslin_inplace43	pnl_vect_create_from_double	
pnl_tridiag_mat_map_inplace41	pnl_vect_create_from_file	
pnl_tridiag_mat_map	pnl_vect_create_from_list	
${ m tridiag\_mat\_inplace}$	pnl_vect_create_from_ptr	
41	pnl_vect_create_from_zero	. 18
pnl_tridiag_mat_minus_double 41	pnl_vect_create_submat	. 29
pnl_tridiag_mat_minus_tridiag_mat41	pnl_vect_create_subvect	. 19
pnl_tridiag_mat_mult_double41	pnl_vect_create_subvect_with_ind	.19
pnl_tridiag_mat_mult_tridiag_mat_term	pnl_vect_cross	. 22
41	pnl_vect_cumprod	
pnl tridiag mat mult vect	pnl vect cumsum	.22
pnl_tridiag_mat_mult_vect	pnl_vect_cumsum	
pnl_tridiag_mat_mult_vect_inplace42	pnl_vect_dist	. 22
pnl_tridiag_mat_mult_vect_inplace42 pnl_tridiag_mat_new40	pnl_vect_dist	. 22 . 21
pnl_tridiag_mat_mult_vect_inplace42 pnl_tridiag_mat_new	pnl_vect_dist  pnl_vect_div_double  pnl_vect_div_vect_term	. 22 . 21 . 21
pnl_tridiag_mat_mult_vect_inplace42 pnl_tridiag_mat_new	pnl_vect_dist	. 22 . 21 . 21 . 22
pnl_tridiag_mat_mult_vect_inplace 42 pnl_tridiag_mat_new40 pnl_tridiag_mat_plus_double41 pnl_tridiag_mat_plus_tridiag_mat41 pnl_tridiag_mat_print41	pnl_vect_dist	. 22 . 21 . 21 . 22 . 22
pnl_tridiag_mat_mult_vect_inplace42pnl_tridiag_mat_new	pnl_vect_dist	. 22 . 21 . 21 . 22 . 22 . 29
pnl_tridiag_mat_mult_vect_inplace42pnl_tridiag_mat_new	pnl_vect_dist  pnl_vect_div_double  pnl_vect_div_vect_term  pnl_vect_eq  pnl_vect_eq_double  pnl_vect_extract_submat  pnl_vect_extract_subvect	. 22 . 21 . 21 . 22 . 22 . 29 . 19
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind	. 22 . 21 . 21 . 22 . 22 . 29 . 19
pnl_tridiag_mat_mult_vect_inplace42pnl_tridiag_mat_new	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 19 . 23
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 19 . 23
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 19 . 23
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find pnl_vect_fprint	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 23 . 20
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 23 . 20 . 20
pnl_tridiag_mat_mult_vect_inplace	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_ pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free	. 22 . 21 . 21 . 22 . 22 . 29 . 19 . 19 . 23 . 20 . 20 . 20 20
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get	. 22 . 21 . 22 . 22 . 29 . 19 . 23 . 20 . 20 . 20 . 20 . 20
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21pnl_vect_clone.19	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get pnl_vect_inv_term	. 22 . 21 . 22 . 22 . 29 . 19 . 23 . 20 . 20 . 20 . 19 20 20 21
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21pnl_vect_clone.19pnl_vect_compact_copy.25	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_ pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_get pnl_vect_get pnl_vect_inv_term pnl_vect_lget	$\begin{array}{c} .\ 22 \\ .\ 21 \\ .\ 22 \\ .\ 22 \\ .\ 29 \\ .\ 19 \\ .\ 23 \\ .\ 20 \\$
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21pnl_vect_clone.19pnl_vect_compact_copy.25pnl_vect_compact_create.25	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get pnl_vect_inv_term pnl_vect_lget pnl_vect_map	$\begin{array}{c} .\ 22 \\ .\ 21 \\ .\ 22 \\ .\ 22 \\ .\ 29 \\ .\ 19 \\ .\ 23 \\ .\ 20 \\ .\ 20 \\ .\ 20 \\ .\ 20 \\ .\ 21 \\ .\ 20 \\ .\ 21 \\ \end{array}$
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21pnl_vect_clone.19pnl_vect_compact_copy.25pnl_vect_compact_create.25pnl_vect_compact_free.26	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get pnl_vect_inv_term pnl_vect_lget pnl_vect_map pnl_vect_map_inplace	$\begin{array}{c} .22\\ .21\\ .22\\ .22\\ .29\\ .19\\ .23\\ .20\\ .20\\ .20\\ .20\\ .21\\ .21\\ .21\\ .$
pnl_tridiag_mat_mult_vect_inplace42pnl_tridiag_mat_new40pnl_tridiag_mat_plus_double41pnl_tridiag_mat_plus_tridiag_mat41pnl_tridiag_mat_print41pnl_tridiag_mat_resize40pnl_tridiag_mat_scalar_prod42pnl_tridiag_mat_set40pnl_tridiag_mat_syslin42pnl_tridiag_mat_syslin_inplace42pnl_tridiag_mat_to_mat40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc12pnl_vect_axpby21pnl_vect_clone.19pnl_vect_compact_copy.25pnl_vect_compact_create.25pnl_vect_compact_free.26pnl_vect_compact_get.26	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get pnl_vect_inv_term pnl_vect_lget pnl_vect_map pnl_vect_map_inplace pnl_vect_map_vect	$\begin{array}{c} .22\\ .21\\ .22\\ .22\\ .29\\ .19\\ .23\\ .20\\ .20\\ .20\\ .20\\ .21\\ .21\\ .21\\ .21\\ .21\\ .21\\ .22\\ .22$
pnl_tridiag_mat_mult_vect_inplace.42pnl_tridiag_mat_new.40pnl_tridiag_mat_plus_double.41pnl_tridiag_mat_plus_tridiag_mat.41pnl_tridiag_mat_print.41pnl_tridiag_mat_resize.40pnl_tridiag_mat_scalar_prod.42pnl_tridiag_mat_set.40pnl_tridiag_mat_syslin.42pnl_tridiag_mat_syslin_inplace.42pnl_tridiag_mat_to_mat.40PNL_TRIDIAGMAT_OBJECT.7pnl_trunc.12pnl_vect_axpby.21pnl_vect_clone.19pnl_vect_compact_copy.25pnl_vect_compact_create.25pnl_vect_compact_free.26	pnl_vect_dist pnl_vect_div_double pnl_vect_div_vect_term pnl_vect_eq pnl_vect_eq_double pnl_vect_extract_submat pnl_vect_extract_subvect pnl_vect_extract_subvect_with_ind pnl_vect_find pnl_vect_fprint pnl_vect_fprint_asrow pnl_vect_fprint_nsp pnl_vect_free pnl_vect_get pnl_vect_inv_term pnl_vect_lget pnl_vect_map pnl_vect_map_inplace	$\begin{array}{c} \cdot 22 \\ \cdot 21 \\ \cdot 21 \\ \cdot 22 \\ \cdot 29 \\ \cdot 19 \\ \cdot 23 \\ \cdot 20 \\ \cdot 20 \\ \cdot 20 \\ \cdot 20 \\ \cdot 21 \end{array}$

pnl_vect_max_index 2	3 pnl_vect_wrap_mat_row30
pnl_vect_min	2 pnl_vect_wrap_subvect19
pnl_vect_min_index2	$3  ext{pnl\_vect\_wrap\_subvect\_with\_last} \dots 19$
pnl_vect_minmax2	
pnl_vect_minmax_index2	3 R
pnl_vect_minus	1 RCadd
pnl_vect_minus_double2	1 RCdiv14
pnl_vect_minus_vect	1 RCmul
pnl_vect_mult_double2	1 RCsub14
pnl_vect_mult_vect_term2	
pnl_vect_new	o D
pnl_vect_norm_infty	$^{\circ}$ SQR
pnl_vect_norm_one 2	2 Structs
pnl_vect_norm_two	PmArray9
PNL_VECT_OBJECT	6 PhiBandMat43
pnl vect permute3	Phibasis03
pnl_vect_permute_inplace3	PhiBicgSolver 48
pnl vect permute inverse	8 Phiceil8
pnl_vect_permute_inverse_inplace 3	PnlCgSolver48
pnl_vect_plus_double	1 Phicmpixrunc
pnl_vect_plus_vect	Pnifunc
pnl_vect_print	n Pnifunc2D
pnl_vect_print_asrow	n Phiruncorunc
pnl_vect_print_nsp	n PniGmresSolver48
pnl_vect_prod	9 Filifiliat40
pnl_vect_qsort	<sub>2</sub> FindmatComplex40
pnl_vect_qsort_index	<sub>3</sub> Риниани
pnl_vect_rand_normal6	1 PhilterationBase 48
pnl_vect_rand_normal_d6	1 Phillist8
pnl_vect_rand_uni	1 Philliat20
pnl_vect_rand_uni_d6	1 PinmarComplex20
pnl_vect_resize	o Philylatint20
pnl_vect_resize_from_ptr1	o PniObject
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pnl_vect_rng_normal	PnIPermutation 38
pnl_vect_rng_normal_d5	Phikheiinck (8
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pnl_vect_rng_uni	FUID.0FU0CD.0012FU0C
pnl_vect_rng_uni_d5	PhiBhrimcBh (8
pnl_vect_scalar_prod	Phikheiinckhijeiinc (8
pnl_vect_set	EURUS 23
pnl_vect_set_double	Entrinagival 59
pnl_vect_set_zero	Pn[TridiagNatLU39
pnl_vect_sum	Phivect
pnl_vect_swap_elements	PHIVECTCOMDACT
pnl_vect_wrap_array	PnlVectComplex
pnl_vect_wrap_hmat4	8 PnlVectInt
pnl vect wrap mat	9