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# Documentation of the pw85 library

*Release 1.1*

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### **Abstract**

This library implements the “contact function” defined by Perram and Wertheim (J. Comp. Phys. 58(3), 409–416, DOI:10.1016/0021-9991(85)90171-8) for two ellipsoids. Given two ellipsoids, this function returns the *square* of the common factor by which both ellipsoids must be scaled (their centers being fixed) in order to be tangentially in contact.

This library is released under a BSD 3-Clause License.



## OVERVIEW

## 1.1 Introduction

It is quite common in materials science to reason on assemblies of ellipsoids as model materials. Although simplified upscaling mean-field/effective-field theories exist for such microstructures, they often fail to capture the finest details of the microstructure, such as orientation correlations between anisotropic inclusions, or particle-size distributions. In order to account for such microstructural details, one must resort to so-called *full-field* numerical simulations (using dedicated tools such as [Damask](#) or [Janus](#), for example).

Full-field simulations require *realizations* of the microstructure. For composites made of ellipsoidal inclusions embedded in a (homogeneous) matrix, this requires to be able to generate assemblies of (non-overlapping) ellipsoids. The basic ingredient of such microstructure simulations is of course the overlap test of two inclusions.

Checking for the overlap (or the absence of it) of two ellipsoids is not as trivial as checking for the overlap of two spheres. Several criteria can be found in the literature [VB72]; [PW85]; [WWK01]; [CYP07]; [ABH18]. We propose an implementation of the *contact function* of Perram and Wertheim [PW85].

The present chapter is organised as follows. We first give a brief description of the contact function. Then, we discuss two essential features of this function: robustness with respect to floating-point errors and suitability for application to Monte-Carlo simulations. Finally, we give a brief description of the pw85 library.

## 1.2 The contact function of Perram and Wertheim [PW85]

The origin being fixed, points are represented by the  $3 \times 1$  column-vector of their coordinates in a global cartesian frame. For  $i = 1, 2$ ,  $E_i \subset \mathbb{R}^3$  denotes the following ellipsoid:

$$(1) \quad E_i = \{m \in \mathbb{R}^3 : (m - c_i)^T \cdot Q_i^{-1} \cdot (m - c_i) \leq 1\},$$

where  $c_i \in \mathbb{R}^3$  is the center of  $E_i$ , and  $Q_i$  is a positive definite matrix. Perram and Wertheim define the following function:

$$(2) \quad f(\lambda; r_{12}, Q_1, Q_2) = \lambda(1-\lambda)r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

where  $0 \leq \lambda \leq 1$  is a scalar,  $Q = (1-\lambda)Q_1 + \lambda Q_2$ , and  $r_{12} = c_2 - c_1$  denotes the center-to-center radius-vector. The *contact function*  $\mu^2(E_1, E_2)$  of the two ellipsoids is defined as the unique maximum of  $f$  over  $(0, 1)$ :

$$(3) \quad \mu^2 = \max\{f(\lambda; r_{12}, Q_1, Q_2), 0 \leq \lambda \leq 1\}.$$

It turns out that the contact function has a simple geometric interpretation. Indeed,  $\mu$  is the quantity by which each of the two ellipsoids  $E_1$  and  $E_2$  must be scaled to bring them in contact. Therefore, an overlap test could be defined as follows

- $\mu^2(E_1, E_2) < 1$ : the two ellipsoids overlap,
- $\mu^2(E_1, E_2) > 1$ : the two ellipsoids do not overlap,
- $\mu^2(E_1, E_2) = 1$ : the two ellipsoids are tangent.

Despite its apparent complexity, this overlap test has two nice features that are discussed below.

## 1.3 Features of the overlap test

### 1.3.1 Robustness with respect to floating-point errors

All overlap tests amount to checking for the sign of a real quantity  $\Phi(E_1, E_2)$  that depends on the two ellipsoids  $E_1$  and  $E_2$ . The ellipsoids do not overlap when  $\Phi(E_1, E_2) < 0$ ; they do overlap when  $\Phi(E_1, E_2) > 0$ . Finally, we usually have  $\Phi(E_1, E_2) = 0$  when  $E_1$  and  $E_2$  are in tangent contact (but it is important to note that, depending on the overlap criterion, the converse is not necessarily true).

In a finite precision setting, we are bound to make wrong decisions about pairs of ellipsoids that are such that  $\Phi$  is small. Indeed, let us consider a pair of ellipsoids  $(E_1, E_2)$  for which the true value of  $\Phi$ ,  $\Phi_e(E_1, E_2)$ , is close to the machine epsilon. Then, the numerical estimate of  $\Phi$ ,  $\Phi_a(E_1, E_2)$ , is also (hopefully) a very small value. However, whether  $\Phi_a(E_1, E_2)$  is the same sign as  $\Phi_e(E_1, E_2)$  (and therefore delivers the correct answer regarding overlap) is uncertain, owing to accumulation of round-off errors. Such misclassifications are acceptable provided that they occur for ellipsoids that are close (nearly in tangent contact). The overlap criterion will be deemed robust if it is such that  $\Phi(E_1, E_2)$  is small for nearly tangent ellipsoids only. This is obviously true of the overlap test based on the contact function of Perram and Wertheim. Note that some of the overlap tests that can be found in the literature do not exhibit such robustness.

### 1.3.2 Application to Monte-Carlo simulations

Generating compact assemblies of hard particles is a notoriously difficult task. Event-driven simulations [DTS05]; [DTS05a] are often used, but require a lot of book-keeping. A comparatively simpler approach [BL13] is similar to atomistic simulations with a non-physical energy. More precisely, starting from an initial configuration where the  $n$  ellipsoids  $E_1, \dots, E_n$  do overlap, a simulated annealing strategy is adopted to minimize the quantity  $U(E_1, \dots, E_n)$  defined as follows:

$$(4) \quad U(E_1, \dots, E_n) = \sum_{1 \leq i < j \leq n} u(E_i, E_j),$$

where  $u(E_1, E_2)$  denotes an *ad-hoc* pair-wise (non-physical) potential, that should vanish when the two ellipsoids do not overlap, and be “more positive when the overlap is greater” (this sentence being deliberately kept vague). A possible choice for  $u$  is the following:

$$(5) \quad u(E_1, E_2) = \max\{0, \mu^{-1}(E_1, E_2)\}.$$

Monte-Carlo simulations using previous implementations of the contact function of Perram and Wertheim and the above definition of the energy of the system were successfully used to produce extremely compact assemblies of ellipsoids [BL13].



## 1.4 Implementation

pw85 is a C library that implements the contact function of Perram and Wertheim. It is released under a BSD-3 license, and is available at <https://github.com/sbrisard/pw85>. It is fully documented at <https://sbrisard.github.io/pw85>.

The core library depends on The [GNU Scientific Library \(GSL\)](#) (for its implementation of the Brent algorithm); the tests also depend on the [GLib](#) and [HDF5](#) libraries.

The API is extremely simple; in particular it defines no custom objects: parameters of all functions are either simple types (`size_t`, `double`) or arrays. Note that all arrays must be pre-allocated and are modified in-place. This minimizes the risk of creating memory leaks when implementing wrappers for higher-level (garbage-collected) languages.

A Python wrapper (based on `ctypes`) is also provided. It has the following (fairly standard) dependencies: [NumPy](#), [pytest](#) and [h5py](#).

Note that when developing the library, several strategies have been tested for the evaluation of the function  $f$  defined above, and its optimization. Evaluation of  $f$  relies on a Cholesky decomposition of  $\mathbf{Q}$ ; we tested the accuracy of this implementation over a comprehensive set of large-precision reference values that are available on Zenodo (<https://doi.org/10.5281/zenodo.3323683>). Optimization of  $f$  first starts with a few iterations of Brent’s robust algorithm. Then, the estimate of the minimizer is refined through a few Newton–Raphson iterations.

## 1.5 Extensions

Several improvements/extensions are planned for this library:

1. Provide a 2D implementation of the contact function.
2. Allow for early stop of the iterations. If, during the iterations, a value of  $\lambda$  is found such that  $f > 1$ , then  $\mu^2$  must be greater than 1, and the ellipsoids certainly do not overlap, which might be sufficient if the user is not interested in the exact value of the contact function.
3. Return error codes when necessary. Note that this would be an extra safety net, as the optimization procedure is extremely robust. Indeed, it never failed for the thousands of test cases considered (the function to optimize has the required convexity over  $(0, 1)$ ).

This project welcomes contributions. We definitely need help for the following points:

1. Define a “Code of conduct”.
2. Improve the Python wrapper (using Cython or a C extension).
3. Implement wrappers for other languages (Julia, Javascript).

## 1.6 Acknowledgements

The author would like to thank Prof. Chloé Arson (GeorgiaTech Institute of Technology, School of Civil and Environmental Engineering) for stimulating exchanges and research ideas that motivated the exhumation of this project (which has long been a defunct Java library).

The author would also like to thank Xianda Shen (GeorgiaTech Institute of Technology, School of Civil and Environmental Engineering) for testing on fruity operating systems the installation procedure of this and related libraries. His dedication led him to valiantly fight long battles with `setuptools` and `brew`.



## INSTALLATION

**Contents**

- *Installing the C library*
- *Building the documentation*
- *Installing the Python bindings*

## 2.1 Installing the C library

The C library depends on

1. The [GLib](#) (for testing purposes)
2. The [GNU Scientific Library \(GSL\)](#) (for the implementation of the Brent algorithm)
3. The [HDF5](#) (for testing purposes)

This is a [CMake](#) based project. The installation procedure is standard. First, clone the repository. Then, cd into the root directory of the pw85 project. Let pw85\_INSTALL\_PREFIX be the path to the directory where pw85 should be installed:

```
$ git clone https://github.com/sbrisard/pw85.git
$ cd pw85
$ mkdir build
$ cd build
$ cmake -DCMAKE_INSTALL_PREFIX=pw85_INSTALL_PREFIX ..
$ cmake --build . --config Release
$ cmake --install . --config Release
```

**Note:** The --config option might not be available, depending on the selected generator.

At this point, pw85 should be installed. You can now run the tests:

```
$ ctest . -C Release
```

**Note:** Depending on the system, you might need to add pw85\_INSTALL\_PREFIX to your PATH environment variable.

To further test your installation, build the example in the [C tutorial](#).

## 2.2 Building the documentation

The documentation of pw85 requires [Sphinx](#). The C++ API docs are built with [Doxygen](#) and the [Breathe](#) extension to [Sphinx](#).

To build the HTML version of the docs in the public subdirectory:

```
$ cd docs
$ sphinx-build -b html . ../public
```

To build the LaTeX version of the docs:

```
$ cd docs
$ make latex
```

## 2.3 Installing the Python bindings

————— **This section to be needed when pybind11 is used.**

To install the pw85 module, cd into the python subdirectory and edit the `setup.cfg` file. Set the `include_dir` and `library_dir` to the appropriate paths. These should be:

```
[pw85]
include_dir = ${CMAKE_INSTALL_PREFIX}/include
library_dir = ${CMAKE_INSTALL_PREFIX}/lib
```

Then, issue the following command:

```
$ python setup.py install --user
```

or (if you intend to edit the project):

```
$ python setup.py develop --user
```

————— **End of this section.**

You need to define the location of the dynamic libraries, for ctypes to be able to import it. This is done through the `pw85.cfg` file, which you must create and place in the following directory

- Windows 10/8/7/Vista: C:\Users\<username>\AppData\Roaming\pw85
- Windows XP/2000: C:\Documents and Settings\<username>\Application Data\pw85
- Mac: /Users/<username>/Library/Application Support/pw85
- Linux: ~/.pw85

(in all cases, the pw85 subdirectory must be created). The contents of the `pw85.cfg` file should be:

```
[pw85]
libpw85 = full/path/to/the/pw85/dynamic/library
libpw85_legacy = full/path/to/the/pw85_legacy/dynamic/library
datadir = full/path/to/the/pw85/data/directory
```

where the `libpw85` and `libpw85_legacy` entries are the full path to the dynamic libraries (\*.dll, \*.so or \*.dylib) *including their name*. All these configure options can be retrieved from the output of `cmake --install ..`. For example, on a Windows machine, where the output was:

```
$ cmake --install .
-- Install configuration: ""
-- Installing: C:/opt/pw85/include/pw85
-- Installing: C:/opt/pw85/include/pw85/pw85.h
-- Installing: C:/opt/pw85/include/pw85/pw85_legacy.h
-- Installing: C:/opt/pw85/lib/libpw85.dll.a
-- Installing: C:/opt/pw85/lib/libpw85.dll
-- Installing: C:/opt/pw85/lib/cmake/pw85/pw85-targets.cmake
-- Installing: C:/opt/pw85/lib/cmake/pw85/pw85-targets-noconfig.cmake
-- Installing: C:/opt/pw85/lib/cmake/pw85/pw85-config.cmake
```

the contents of `pw85.cfg` is:

```
[pw85]
libpw85 = C:/opt/pw85/lib/libpw85.dll
libpw85_legacy = C:/opt/pw85/lib/libpw85_legacy.dll
datadir = C:/opt/pw85/share/pw85
```

To run the tests with [Pytest](#):

```
$ python -m pytest tests/test_pw85.py
```

You can also test the “legacy” API. This requires the [h5py](#) module. To run the tests, issue the command:

```
$ python -m pytest tests/test_pw85_legacy.py
```

(beware, these tests take some time!).



## TUTORIAL

### Contents

- *Python tutorial*
  - *Checking the output*
- *C tutorial*

In this tutorial, we consider two ellipsoids, and check whether or not they overlap.

Ellipsoid  $E_1$  is an [oblate spheroid](#) centered at point  $x_1 = (-0.5, 0.4, -0.7)$ , with equatorial radius  $a_1 = 10$ , polar radius  $c_1 = 0.1$  and polar axis  $(0, 0, 1)$ .

Ellipsoid  $E_2$  is a [prolate spheroid](#) centered at point  $(0.2, -0.3, 0.4)$ , with equatorial radius  $a_1 = 0.5$ , polar radius  $c_1 = 5$  and polar axis  $(1, 0, 0)$ .

To carry out the overlap check, we must first create the representation of ellipsoids  $E_i$  as quadratic forms  $Q_i$  (see [Mathematical representation of ellipsoids](#)). Convenience functions are provided to compute the matrix representation of a *spheroid*.

---

**Note:** In principle, the contact function implemented in PW85 applies to *any* ellipsoids (with unequal axes). However, at the time of writing this tutorial (2019-01-01), convenience functions to compute the matrix representation of a general ellipsoid is not yet implemented. Users must compute the matrices themselves.

---

We first check for the overlap of  $E_1$  and  $E_2$  using the Python wrapper of pw85. We will then illustrate the C API.

### 3.1 Python tutorial

The Python module relies on [NumPy](#) for passing arrays to the underlying C library. We therefore import both modules:

```
>>> import numpy as np
>>> import pw85
```

and define the parameters of the simulation:

```
>>> x1 = np.array([-0.5, 0.4, -0.7])
>>> n1 = np.array([0., 0., 1.])
>>> a1, c1 = 10, 0.1
>>> x2 = np.array([0.2, -0.3, 0.4])
```

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```
>>> n2 = np.array([1., 0., 0.])
>>> a2, c2 = 0.5, 5.
>>> r12 = x2-x1
```

where  $r_{12}$  is the vector that joins the center of the first ellipsoid,  $x_1$ , to the center of the second ellipsoid,  $x_2$ .

We use the function `pw85.spheroid()` to create the matrix representations  $q_1$  and  $q_2$  of the two ellipsoids:

```
>>> q1 = pw85.spheroid(a1, c1, n1)
>>> q1
array([ 1.e+02, -0.e+00, -0.e+00,  1.e+02, -0.e+00,  1.e-02])
>>> q2 = pw85.spheroid(a2, c2, n2)
>>> q2
array([25. ,  0. ,  0. ,  0.25,  0. ,  0.25])
```

We can now compute the value of the contact function — see the documentation of `pw85.contact_function()`:

```
>>> mu2, lambda_ = pw85.contact_function(r12, q1, q2)
>>> print('μ² = {}'.format(mu2))
>>> print('λ = {}'.format(lambda_))
μ² = 3.362706040638343
λ = 0.1668589553405904
```

We find that  $\mu^2 > 1$ , hence  $\mu > 1$ . In other words, both ellipsoids must be *swollen* in order to bring them in contact: the ellipsoids do not overlap!

### 3.1.1 Checking the output

The output of this simulation can readily be checked. First, we can check that  $q_1$  and  $q_2$  indeed represent the ellipsoids  $E_1$  and  $E_2$ . To do so, we first construct the symmetric matrices  $Q_1$  and  $Q_2$  from their upper triangular part

```
>>> Q1 = np.zeros((3, 3), dtype=np.float64)
>>> i, j = np.triu_indices_from(Q1)
>>> Q1[i, j] = q1
>>> Q1[j, i] = q1
>>> Q1
array([[ 1.e+02, -0.e+00, -0.e+00],
       [-0.e+00,  1.e+02, -0.e+00],
       [-0.e+00, -0.e+00,  1.e-02]])
```

```
>>> Q2 = np.zeros_like(Q1)
>>> Q2[i, j] = q2
>>> Q2[j, i] = q2
>>> Q2
array([[25. ,  0. ,  0. ],
       [ 0. ,  0.25,  0. ],
       [ 0. ,  0. ,  0.25]])
```

We can now check these matrices for some remarkable points, first for ellipsoid  $E_1$

```
>>> Q1_inv = np.linalg.inv(Q1)
>>> f1 = lambda x: Q1_inv.dot(x).dot(x)
>>> f1((a1, 0., 0.))
1.0
>>> f1((-a1, 0., 0.))
```

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```

1.0
>>> f1((0., a1, 0.))
1.0
>>> f1((0., -a1, 0.))
1.0
>>> f1((0., 0., c1))
0.9999999999994884
>>> f1((0., 0., -c1))
0.9999999999994884

```

then for ellipsoid  $E_2$

```

>>> Q2_inv = np.linalg.inv(Q2)
>>> f2 = lambda x: Q2_inv.dot(x).dot(x)
>>> f2((c2, 0., 0.))
1.0
>>> f2((-c2, 0., 0.))
1.0
>>> f2((0., a2, 0.))
1.0
>>> f2((0., -a2, 0.))
1.0
>>> f2((0., 0., a2))
1.0
>>> f2((0., 0., -a2))
1.0

```

Note that in the above tests, we have omitted the centers of ellipsoids  $E_1$  et  $E_2$  (both ellipsoids were translated to the origin).

We will now verify the correctness of the value found for the scaling factor  $\mu$ . To do so, we will find the coordinates of the contact point of the two scaled ellipsoids, and check that the normals to the two ellipsoids at that point coincide.

Although we use formulæ from the [Theory](#) section to find the coordinates of the contact point,  $x_0$ , it is not essential for the time being to fully understand this derivation. What really matters is to check that the resulting point  $x_0$  is indeed the contact point of the two scaled ellipsoids; how the coordinates of this point were found is irrelevant.

From the value of  $\lambda$  returned by the function `pw85.contact_function()`, we compute  $Q$  defined by Eq. (10) in section [Theory](#), as well as  $x = Q^{-1} \cdot r_{12}$

```

>>> Q = (1-lambda_)*Q1+lambda_*Q2
>>> x = np.linalg.solve(Q, r12)

```

From which we find  $x_0$ , using either Eq. (9a) or Eq. (9b) (and we can check that both give the same result)

```

>>> x0a = x1+(1-lambda_)*np.dot(Q1, x)
>>> x0a
array([ 0.16662271, -0.29964969, -0.51687799])
>>> x0b = x2-lambda_*np.dot(Q2, x)
>>> x0b
array([ 0.16662271, -0.29964969, -0.51687799])

```

We can now check that  $x_0$  belongs to the two scaled ellipsoids, that we first define, overriding the matrices of the unscaled ellipsoids, that are no longer needed. We observe that if ellipsoid  $E_i$  is scaled by  $\mu$ , then its matrix representation  $Q_i$  is scaled by  $\mu^2$ , and its inverse  $Q_i^{-1}$  is scaled by  $\mu^{-2}$ .

```
>>> x0 = x0a
>>> Q1 *= mu2
>>> Q2 *= mu2
>>> Q1_inv /= mu2
>>> Q2_inv /= mu2
```

```
>>> x = x0-x1
>>> Q1_inv.dot(x).dot(x)
1.00000000000058238
```

```
>>> x = x0-x2
>>> Q2_inv.dot(x).dot(x)
0.99999999999988334
```

Therefore  $x_0$  indeed belongs to both ellipsoids. We now compute the normal  $n_i$  to ellipsoid  $E_i$  at point  $x_0$ . Since ellipsoid  $E_i$  is defined by the level-set:  $(x-x_i)^T \cdot Q_i^{-1} \cdot (x-x_i) = 1$ , the normal to  $E_i$  is given by  $Q_i^{-1} \cdot (x-x_i)$  (which is then suitably normalized)

```
>>> n1 = Q1_inv.dot(x0-x1)
>>> n1 /= np.linalg.norm(n1)
>>> n1
array([ 3.64031943e-04, -3.82067448e-04,  9.99999861e-01])
```

```
>>> n2 = Q2_inv.dot(x0-x2)
>>> n2 /= np.linalg.norm(n2)
>>> n2
array([-3.64031943e-04,  3.82067448e-04, -9.99999861e-01])
```

We find that  $n_1 = -n_2$ . Therefore,  $E_1$  and  $E_2$  are in external contact. QED

Follow this link to download the above Python script.

## 3.2 C tutorial

The Python interface to PW85 has been kept close to the underlying C API. The following C program (download source file) defines the two ellipsoids, then computes  $\mu^2$  and  $\lambda$ :

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

#include "pw85/pw85.h"

#define DIM 3
#define SYM 6

int main() {
    double x1[] = {-0.5, 0.4, -0.7};
    double n1[] = {0., 0., 1.};
    double a1 = 10.;
    double c1 = 0.1;

    double x2[] = {0.2, -0.3, 0.4};
    double n2[] = {1., 0., 0.};
    double a2 = 0.5;
```

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```

double c2 = 5.;

double r12[DIM];
for (int i = 0; i < DIM; i++) r12[i] = x2[i] - x1[i];

double q1[SYM], q2[SYM];
pw85_spheroid(a1, c1, n1, q1);
pw85_spheroid(a2, c2, n2, q2);

double out[2];
pw85_contact_function(r12, q1, q2, out);
printf("mu^2 = %g\n", out[0]);
printf("lambda = %g\n", out[1]);
printf("\n");
}

```

A CMakeLists.txt file is provided for the compilation of the tutorial using the [CMake](#). You can reuse it in one of your own projects (download):

```

cmake_minimum_required(VERSION 3.13)

project("tutorial")

find_package(GSL REQUIRED)
find_package(pw85 CONFIG REQUIRED)

add_executable(${PROJECT_NAME} ${PROJECT_NAME}.c)
target_link_libraries(${PROJECT_NAME} pw85)

```

cd into the c\_tutorial subdirectory. The provided example program should be compiled and linked against pw85:

```

$ mkdir build
$ cd build
$ cmake -Dpw85_DIR=pw85_INSTALL_PREFIX/lib/cmake/pw85 ..
$ cmake --build . --config Release

```

An executable called tutorial should be present in the build/Release subdirectory. On execution, it prints the following lines to stdout:

```

mu^2 = 3.36271
lambda = 0.166859

```



### Contents

- *Mathematical representation of ellipsoids*
- *The contact function of two ellipsoids*
- *Geometric interpretation*

This chapter provides the theoretical background to the Perram–Wertheim algorithm [PW85]. We use matrices rather than tensors: a point/vector is therefore defined through the  $3 \times 1$  column-vector of its coordinates. Likewise, a second-rank tensor is represented by its  $3 \times 3$  matrix.

Only the global, cartesian frame is considered here, and there is no ambiguity about the basis to which these column vectors and square matrices refer.

## 4.1 Mathematical representation of ellipsoids

Ellipsoids are defined from their center  $c$  and a positive-definite quadratic form  $Q$  as the set of points  $m$  such that:

$$(1) \quad (m-c)^T \cdot Q^{-1} \cdot (m-c) \leq 1.$$

$Q$  is a symmetric, positive-definite matrix:

$$(2) \quad Q = \sum_i a_i^2 v_i \cdot v_i^T,$$

where  $a_1, a_2, a_3$  are the lengths of the principal semi-axes and  $v_1, v_2, v_3$  their directions (unit vectors).

In the PW85 library,  $Q$  is represented as a `double[6]` array `q` which stores the upper triangular part of  $Q$  in row-major order:

$$(3) \quad Q = \begin{bmatrix} q[0] & q[1] & q[2] \\ & q[3] & q[4] \\ \text{sym.} & & q[5] \end{bmatrix}.$$

## 4.2 The contact function of two ellipsoids

Let  $E_1$  and  $E_2$  be two ellipsoids, defined by their centers  $c_1$  and  $c_2$  and quadratic forms  $Q_1$  and  $Q_2$ , respectively.

For  $0 \leq \lambda \leq 1$  and a point  $x$ , we introduce the function:

$$(4) \quad F(x, \lambda) = \lambda(x - c_1)^T \cdot Q_1^{-1} \cdot (x - c_1) + (1 - \lambda)(x - c_2)^T \cdot Q_2^{-1} \cdot (x - c_2).$$

For fixed  $\lambda$ ,  $F(x, \lambda)$  has a unique minimum [PW85]  $f(\lambda)$ , and we define:

$$(5) \quad f(\lambda) = \min\{ F(x, \lambda), x \in \mathbb{R}^3 \}, \quad 0 \leq \lambda \leq 1.$$

Now, the function  $f$  has a unique maximum over  $[0, 1]$ , and the “contact function”  $F(r_{12}, Q_1, Q_2)$  of ellipsoids  $E_1$  and  $E_2$  is defined as:

$$(6) \quad F(r_{12}, Q_1, Q_2) = \max\{ f(\lambda), 0 \leq \lambda \leq 1 \},$$

where  $r_{12} = c_2 - c_1$ . It can be shown that

- if  $F(r_{12}, Q_1, Q_2) < 1$  then  $E_1$  and  $E_2$  overlap,
- if  $F(r_{12}, Q_1, Q_2) = 1$  then  $E_1$  and  $E_2$  are externally tangent,
- if  $F(r_{12}, Q_1, Q_2) > 1$  then  $E_1$  and  $E_2$  do not overlap.

The contact function therefore provides a criterion to check overlap of two ellipsoids. The PW85 library computes this value.

## 4.3 Geometric interpretation

The scalar  $\lambda$  being fixed, we introduce the minimizer  $x_0(\lambda)$  of  $F(x, \lambda)$ . The stationarity of  $F$  w.r.t to  $x$  reads:

$$(7) \quad \nabla F(x_0(\lambda), \lambda) = 0,$$

which leads to:

$$(8) \quad \lambda Q_1^{-1} \cdot [x_0(\lambda) - c_1] + (1 - \lambda) Q_2^{-1} \cdot [x_0(\lambda) - c_2] = 0,$$

and can be rearranged:

$$(9a) \quad x_0(\lambda) - c_1 = (1 - \lambda) Q_1 \cdot Q^{-1} \cdot r_{12},$$

$$(9b) \quad x_0(\lambda) - c_2 = -\lambda Q_2 \cdot Q^{-1} \cdot r_{12},$$

with:

$$(10) \quad Q = (1 - \lambda) Q_1 + \lambda Q_2.$$

It results from the above that:

$$(11) \quad f(\lambda) = F(x_0(\lambda), \lambda) = \lambda(1 - \lambda) r_{12}^T \cdot Q^{-1} \cdot r_{12}.$$

Maximization of  $f$  with respect to  $\lambda$  now delivers the stationarity condition:

$$(12) \quad 0 = f'(\lambda) = \nabla F(x_0(\lambda), \lambda) \cdot x_0'(\lambda) + \frac{\partial F}{\partial \lambda}(x_0(\lambda), \lambda).$$

Using Eqs. (4) and (7), it is found that  $f$  is minimum for  $\lambda = \lambda_0$  such that:

$$(13) \quad [x_0(\lambda_0) - c_1]^T \cdot Q_1^{-1} \cdot [x_0(\lambda_0) - c_1] = [x_0(\lambda_0) - c_2]^T \cdot Q_2^{-1} \cdot [x_0(\lambda_0) - c_2].$$

Let  $\mu^2$  be this common value. It trivially results from Eqs. (4) and (13) that  $\mu^2 = F(x_0(\lambda_0), \lambda_0)$ . In other words,  $\mu^2$  is the value of the contact function.

We are now in a position to give a geometric interpretation of  $\mu$ . It results from Eq. (13) and the definition of  $\mu$  that:

$$(14a) \quad [x_0(\lambda_0) - c_1]^T \cdot (\mu^2 Q_1)^{-1} \cdot [x_0(\lambda_0) - c_1] = 1,$$

and:

$$(14b) \quad [x_0(\lambda_0) - c_2]^T \cdot (\mu^2 Q_2)^{-1} \cdot [x_0(\lambda_0) - c_2] = 1.$$

The above equations mean that  $x_0(\lambda_0)$  belongs to both ellipsoids centered at  $c_j$  and defined by the symmetric, positive-definite quadratic form  $\mu^2 Q_j$  ( $j = 1, 2$ ). These two ellipsoids are nothing but the initial ellipsoids  $E_1$  and  $E_2$ , scaled by the *same* factor  $\mu$ .

Furthermore, Eq. (8) applies for  $\lambda = \lambda_0$ . Therefore, the normals to the scaled ellipsoids coincide at  $x_0(\lambda_0)$ : the two scaled ellipsoids are externally tangent.

To sum up,  $\mu$  is the common factor by which ellipsoids  $E_1$  and  $E_2$  must be scaled in order for them to be externally tangent at point  $x_0(\lambda_0)$ .





## IMPLEMENTATION OF THE FUNCTION $f$

In this chapter, we explain how the contact function is computed. From Eq. (12) in chapter *Theory*, the value of the contact function is found from the solution  $\lambda$  to equation  $f'(\lambda) = 0$ , where it is recalled that  $f$  is defined as follows:

$$(1) \quad f(\lambda) = \lambda(1-\lambda) r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

with:

$$(2) \quad Q = (1-\lambda)Q_1 + \lambda Q_2.$$

In the present chapter, we discuss two implementations for the evaluation of  $f$ . The *first implementation* uses the Cholesky decomposition of  $Q$ . The *second implementation* uses a representation of  $f$  as a quotient of two polynomials (rational fraction).

### 5.1 Implementation #1: using Cholesky decompositions

Since  $Q$  is a symmetric, positive definite matrix, we can compute its *Cholesky decomposition*, which reads as follows:

$$(3) \quad Q = L \cdot L^T,$$

where  $L$  is a lower-triangular matrix. Using this decomposition, it is straightforward to compute  $s = Q^{-1} \cdot r$  (where we write  $r$  as a shorthand for  $r_{12}$ ), so that:

$$(4) \quad f(\lambda) = \lambda(1-\lambda) r^T \cdot s.$$

In order to solve  $f'(\lambda) = 0$  numerically, we use a *Newton–Raphson* procedure, which requires the first and second derivatives of  $f$ . It is readily found that:

$$(5) \quad s' = -Q^{-1} \cdot Q' \cdot Q^{-1} \cdot r = -Q^{-1} \cdot u \quad \text{and} \quad r^T \cdot s' = -r^T \cdot Q^{-1} \cdot u = -s^T \cdot u,$$

with  $u = Q_{12} \cdot s$  and  $Q_{12} = Q_2 - Q_1$ . Therefore:

$$(6) \quad f'(\lambda) = (1-2\lambda) r^T \cdot s - \lambda(1-\lambda) s^T \cdot u.$$

Similarly, introducing  $v = Q^{-1} \cdot u$ :

$$(7) \quad s^T \cdot u' = s^T \cdot Q_{12} \cdot s' = -s^T \cdot Q_{12} \cdot Q^{-1} \cdot u = -u^T \cdot v,$$

and:

$$(8) \quad u^T \cdot s' = -u^T \cdot Q^{-1} \cdot u = -u^T \cdot v.$$

Therefore:

$$(9) \quad f''(\lambda) = -2r^T \cdot s - 2(1-2\lambda)s^T \cdot u + 2\lambda(1-\lambda)u^T \cdot v.$$

## 5.2 Implementation #2: using rational functions

We observe that  $f(\lambda)$  is a rational function [see Eq. (1)], and we write:

$$(10) \quad f(\lambda) = \frac{\lambda(1-\lambda)a(\lambda)}{b(\lambda)},$$

with:

$$(11a) \quad a(\lambda) = r_{12}^T \cdot \text{adj}[(1-\lambda)Q_1 + \lambda Q_2] \cdot r_{12} = a_0 + a_1\lambda + a_2\lambda^2,$$

$$(11b) \quad b(\lambda) = \det[(1-\lambda)Q_1 + \lambda Q_2] = b_0 + b_1\lambda + b_2\lambda^2 + b_3\lambda^3,$$

where  $\text{adj}(Q)$  denotes the adjugate matrix of  $Q$  (transpose of its cofactor matrix), see e.g. [Wikipedia](#).

The coefficients  $a_i$  and  $b_i$  are found from the evaluation of  $a(\lambda)$  and  $b(\lambda)$  for specific values of  $\lambda$ :

$$(12a) \quad a_0 = a(0),$$

$$(12b) \quad a_1 = \frac{a(1) - a(-1)}{2},$$

$$(12c) \quad a_2 = \frac{a(1) + a(-1)}{2} - a(0),$$

$$(12d) \quad b_0 = b(0),$$

$$(12e) \quad b_1 = \frac{8b(\frac{1}{2})}{3} - 2b(0) - \frac{b(1)}{2} - \frac{b(-1)}{6}$$

$$(12f) \quad b_2 = \frac{b(1) + b(-1)}{2} - b(0),$$

$$(12g) \quad b_3 = -\frac{8b(\frac{1}{2})}{3} + 2b(0) + b(1) - \frac{b(-1)}{3}.$$

This requires the implementation of the determinant and the adjugate matrix of a  $3 \times 3$ , symmetric matrix, see `pw85__det_sym()` and `pw85__xT_adjA_x()`.

Evaluating the derivative of  $f$  with respect to  $\lambda$  is fairly easy. The following [SymPy](#) script will do the job:

```
import sympy

from sympy import Equality, numer, pprint, Symbol

if __name__ == '__main__':
    sympy.init_printing(use_latex=False, use_unicode=True)
```

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```

λ = Symbol('λ')
a = sum(sympy.Symbol('a{}'.format(i))*λ**i for i in range(3))
b = sum(sympy.Symbol('b{}'.format(i))*λ**i for i in range(4))
f = λ*(1-λ)*a/b
f_prime = f.diff(λ).ratsimp()
c = numer(f_prime)
c_dict = c.collect(λ, evaluate=False)
for i in range(sympy.degree(c, gen=λ)+1):
    pprint(Equality(Symbol('c{}'.format(i)), c_dict[λ**i]))

```

It is readily found that:

$$(13) \quad f'(\lambda) = \frac{c(\lambda)}{b(\lambda)^2},$$

where  $c(\lambda)$  is a sixth-order polynomial in  $\lambda$ :

$$(14) \quad c(\lambda) = c_0 + c_1\lambda + c_2\lambda^2 + c_3\lambda^3 + c_4\lambda^4 + c_5\lambda^5 + c_6\lambda^6,$$

with:

$$\begin{aligned}
 (15a) \quad c_0 &= a_0b_0, \\
 (15b) \quad c_1 &= 2(a_1-a_0)b_0, \\
 (15c) \quad c_2 &= -a_0(b_1+b_2) + 3b_0(a_2-a_1) + a_1b_1, \\
 (15d) \quad c_3 &= 2[b_1(a_2-a_1) - a_0b_3] - 4a_2b_0, \\
 (15e) \quad c_4 &= (a_0-a_1)b_3 + (a_2-a_1)b_2 - 3a_2b_1, \\
 (15f) \quad c_5 &= -2a_2b_2, \\
 (15g) \quad c_6 &= -a_2b_3,
 \end{aligned}$$

Solving  $f'(\lambda) = 0$  for  $\lambda$  is therefore equivalent to finding the unique root of  $c$  in the interval  $0 \leq \lambda \leq 1$ . For the sake of robustness, the `bisection method` has been implemented (more efficient methods will be implemented in future versions).

Once  $\lambda$  is found,  $\mu$  is computed from  $\mu^2 = f(\lambda)$  using Eq. (10).

## 5.3 Comparison of the two implementations

High precision reference data was generated using the `mpmath` library. The reference dataset is fully described and freely downloadable from the [Zenodo platform](https://zenodo.org/doi/10.5281/zenodo.3323683) (DOI:10.5281/zenodo.3323683). Accuracy of both implementations is then evaluated through the following script (download source file):

```

#include <glib.h>
#include < hdf5.h>
#include < hdf5_hl.h>
#include < pw85.h>
#include < pw85_legacy.h>

void read_dataset_double(hid_t const hid, char const *dset_name, size_t *size,
                        double **buffer) {
    int ndims;
    H5LTget_dataset_ndims(hid, dset_name, &ndims);
    hsize_t *dim = g_new(hsize_t, ndims);
    H5LTget_dataset_info(hid, dset_name, dim, NULL, NULL);

```

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```

*size = 1;
for (size_t i = 0; i < ndims; i++) {
    *size *= dim[i];
}
*buffer = g_new(double, *size);
H5LTread_dataset_double(hid, dset_name, *buffer);
g_free(dim);
}

void update_histogram(double act, double exp, size_t num_bins, size_t *hist) {
    double const err = fabs((act - exp) / exp);
    int prec;
    if (err == 0.0) {
        prec = num_bins - 1;
    } else {
        prec = (int)(floor(-log10(err)));
        if (prec <= 0) {
            prec = 0;
        }
        if (prec >= num_bins) {
            prec = num_bins - 1;
        }
    }
    ++hist[prec];
}

int main() {
    hid_t const hid = H5Fopen(PW85_REF_DATA_PATH, H5F_ACC_RDONLY, H5P_DEFAULT);

    size_t num_directions;
    double *directions;
    read_dataset_double(hid, "/directions", &num_directions, &directions);
    num_directions /= PW85_DIM;

    size_t num_lambdas;
    double *lambdas;
    read_dataset_double(hid, "/lambdas", &num_lambdas, &lambdas);

    size_t num_radai;
    double *radai;
    read_dataset_double(hid, "/radai", &num_radai, &radai);

    size_t num_spheroids;
    double *spheroids;
    read_dataset_double(hid, "/spheroids", &num_spheroids, &spheroids);
    num_spheroids /= PW85_SYM;

    size_t num_expecteds;
    double *expecteds;
    read_dataset_double(hid, "/F", &num_expecteds, &expecteds);

    double *exp = expecteds;
    double params[2 * PW85_SYM + PW85_DIM];

    size_t num_bins = 16;
    size_t hist1[num_bins];
    size_t hist2[num_bins];

```

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```

for (size_t i = 0; i < num_bins; i++) {
    hist1[i] = 0;
    hist2[i] = 0;
}
for (size_t i1 = 0; i1 < num_spheroids; i1++) {
    memcpy(params + PW85_DIM, spheroids + PW85_SYM * i1,
           PW85_SYM * sizeof(double));
    for (size_t i2 = 0; i2 < num_spheroids; i2++) {
        memcpy(params + PW85_DIM + PW85_SYM, spheroids + PW85_SYM * i2,
               PW85_SYM * sizeof(double));
        for (size_t i = 0; i < num_directions; i++) {
            memcpy(params, directions + PW85_DIM * i, PW85_DIM * sizeof(double));
            for (size_t j = 0; j < num_lambdas; j++, exp++) {
                double const act1 = -pw85_f_neg(lambdas[j], params);
                update_histogram(act1, *exp, num_bins, hist1);
                double out[2];
                pw85_legacy_f2(lambdas[j], params, params + PW85_DIM,
                              params + PW85_DIM + PW85_SYM, out);
                double const act2 = out[0];
                update_histogram(act2, *exp, num_bins, hist2);
            }
        }
    }
}

FILE *f = fopen(HISTOGRAM_PATH, "w");
for (size_t i = 0; i < num_bins; i++) {
    fprintf(f, "%d,%g,%g\n", (int)i,
           100. * ((double)hist1[i]) / ((double)num_expecteds),
           100. * ((double)hist2[i]) / ((double)num_expecteds));
}
fclose(f);

g_free(spheroids);
g_free(radii);
g_free(lambdas);
g_free(directions);
H5Fclose(hid);

return 0;
}

```

**Note:** To compute this program, you might need to pass the options `-Dpw85_include=...`, `-Dpw85_lib=...` and `-Dpw85_data=...` to meson (see [C tutorial](#)).

We get the histograms shown in [Fig. 5.1](#). These histograms show that *Implementation #1* is more accurate than *Implementation #2*. The former will therefore be selected as default.

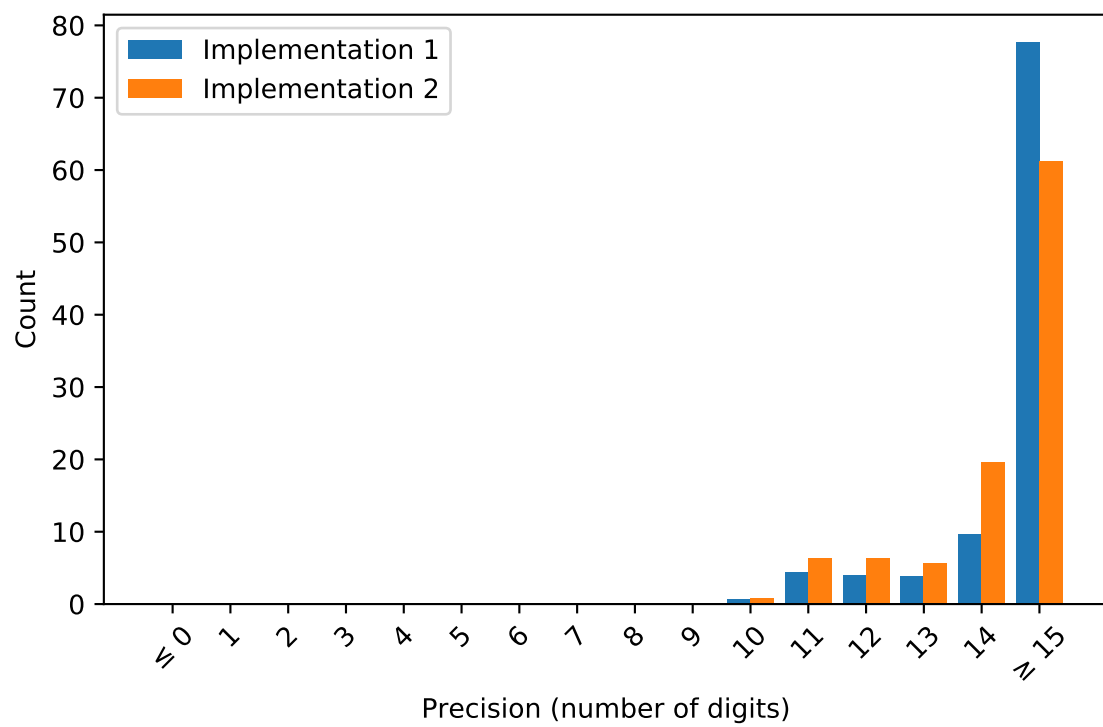


Fig. 5.1: Accuracy of the two implementations.

## OPTIMIZATION OF THE FUNCTION $f$

It was shown in chapter *Theory* [see Eq. (6)] that the contact function was defined as the maximum for  $0 \leq \lambda \leq 1$  of the function  $f$  discussed in chapter *Implementation of the function  $f$* .

Given that the first and second derivatives of  $f$  can be computed explicitly (see section *Implementation #1: using Cholesky decompositions* in chapter *Implementation of the function  $f$* ) it would be tempting to use the Newton–Raphson method to solve  $f'(\lambda)$  iteratively. However, our experiments show that this method performs very poorly in the present case, because the variations of  $f$  can be quite sharp in the neighborhood of  $\lambda = 0$  or  $\lambda = 1$ . To carry out the optimization of  $f$ , we therefore proceed in two steps.

In the first step, we use a robust optimization algorithm. We selected here *Brent’s method*, as implemented in the *GNU Scientific Library (GSL)*. However, this method delivers a relatively low accuracy of the maximizer and the maximum.

Therefore, in the second step, we use a few Newton–Raphson iterations to refine the previously obtained estimates of the minimizer and minimum of  $f$ . In the remainder of this chapter, we describe how these Newton–Raphson iterations are performed.

Our starting point is Eqs. (9) and (13) in chapter *Theory*, from which it results that for a given value of  $\lambda$  we can define two values of  $\mu^2$ : one is provided by Eq. (9a), the other one is given by Eq. (9b) (both in chapter *Theory*):

$$\begin{aligned} (1a) \quad \mu_1^2 &= [x_0(\lambda_0) - c_1]^T \cdot Q_1^{-1} \cdot [x_0(\lambda_0) - c_1] = (1-\lambda)^2 s^T \cdot Q_1 \cdot s, \\ (1b) \quad \mu_2^2 &= [x_0(\lambda_0) - c_2]^T \cdot Q_2^{-1} \cdot [x_0(\lambda_0) - c_2] = \lambda^2 s^T \cdot Q_2 \cdot s, \end{aligned}$$

where we have introduced  $s = Q^{-1} \cdot r_{12}$ . We further define the matrix  $Q_{12} = Q_2 - Q_1$ , so that:

$$(2) \quad Q_1 = Q - \lambda Q_{12} \quad \text{and} \quad Q_2 = Q + (1-\lambda) Q_{12}.$$

Combining Eqs. (1) and (2) and recalling that  $Q \cdot s = r$  then delivers the following expressions:

$$\begin{aligned} (3a) \quad \mu_1^2 &= (1-\lambda)^2 r^T \cdot s - \lambda(1-\lambda)^2 s^T \cdot u, \\ (3b) \quad \mu_2^2 &= \lambda^2 r^T \cdot s + \lambda^2(1-\lambda) s^T \cdot u, \end{aligned}$$

where we have introduced  $u = Q_{12} \cdot s$ .

The above expressions seem to behave slightly better from a numerical point of view. Our problem is now to find  $\lambda$  such that  $\mu_1^2 = \mu_2^2$ . We therefore define the following residual:

$$(4) \quad g(\lambda) = \mu_2^2 - \mu_1^2 = (2\lambda-1) r^T \cdot s + \lambda(1-\lambda) s^T \cdot u,$$

and we need to find  $\lambda$  such that  $g(\lambda) = 0$ . In order to implement Newton–Raphson iterations, we need the expression of the derivative of the residual. Using results that are presented in section *Implementation #1: using Cholesky decompositions*, we readily find that:

$$(5) \quad g'(\lambda) = 2r^T \cdot s + 2(1-2\lambda) s^T \cdot u - 2\lambda(1-\lambda) u^T \cdot v.$$

Eqs. (4) and (5) are then used for the final, refinement step of determination of  $\lambda$ .



## TESTING THE IMPLEMENTATION OF THE CONTACT FUNCTION

This chapter describes how our implementation of the contact function is tested. The source of the unit tests can be found in the file `src/test_pw85.c`. Note that the tests described here are repeated over a large set of tests case, including very flat and very slender spheroids, for various relative orientations and center-to-center distances.

In the present chapter, we assume that the two ellipsoids (their matrices  $Q_1$  and  $Q_2$  are given), as well as their center-to-center radius vector  $r_{12}$ . Then, a call to `pw85_contact_function()` delivers an estimate of  $\lambda$  and  $\mu^2$ .

We first assert that  $\mu_1^2$  and  $\mu_2^2$  as defined by Eq. (3) in chapter *Optimization of the function  $f$*  are close to the value returned by `pw85_contact_function()`. For all the cases considered here, this is true up to a relative error of  $10^{-10}$ .

We also check that  $f'(\lambda) = 0$ , up to an absolute error of  $\Delta\lambda f''(\lambda)$  where  $\Delta\lambda$  is the absolute tolerance on  $\lambda$  for the stopping criterion of the Brent iterations, as defined by the macro `PW85_LAMBDA_ATOL`.

---

**Note:** The PW85 library offers a “new” API and a “legacy” API. The latter is kept for reference. The new API is generally more accurate and robust, and should be preferred by most users. Both APIs are thoroughly tested; however, we adopted two different testing strategies.

The legacy API is solely (but fully) tested through its Python wrapper using `pytest`.

The new API is fully tested through pure C tests (using `GLib`). Then the Python wrapper is also tested (using `pytest`). However, the python tests do not need to be as thorough, since only the validity of the wrapper itself must be checked, not the validity of the underlying C library.

---



## THE C API

### Contents

- *Representation of vectors and matrices*
- *The new API*
- *The “legacy” API*

---

**Note:** we use the following naming convention

- “public” functions are prefixed with `pw85_` or `pw85_legacy_` (single underscore),
- “private” functions are prefixed with `pw85__` or `pw85_legacy__` (double underscore).

Note that “public” and “private” is a matter of convention here, since all functions are exposed (mostly, for testing purposes). However, double underscored functions should not be considered as part of the public API and should not be used, since they are susceptible of incompatible changes (or even removal) in future versions.

---

## 8.1 Representation of vectors and matrices

An ellipsoid is defined from its center  $c$  (a  $3 \times 1$ , column-vector) and quadratic form  $Q$  (a  $3 \times 3$ , symmetric, positive definite matrix) as the set of points  $m$  such that:

$$(m - c)^T \cdot Q^{-1} \cdot (m - c) \leq 1.$$

In this module, objects referred to as “vectors” are `double[3]` arrays of coordinates. In other words, the representation of the vector  $x$  is the `double[3]` array  $x$  such that:

$$x = \begin{bmatrix} x[0] \\ x[1] \\ x[2] \end{bmatrix}.$$

Objects referred to as “symmetric matrices” (or “quadratic forms”) are of type `double[6]`. Such arrays list in row-major order the coefficients of the triangular upper part. In other words, the representation of a the symmetric matrix  $A$  is the `double[6]` array  $a$  such that:

$$A = \begin{bmatrix} a[0] & a[1] & a[2] \\ & a[3] & a[4] \\ \text{sym.} & & a[5] \end{bmatrix}.$$

## 8.2 The new API

The functions and macros gathered below form the new API that should be invoked by most users. To use these functions and macros in your code, you must include the following header:

```
#include <pw85.h>
```

and use the following link directive:

```
-lpw85
```

### PW85\_VERSION

The current version of the library.

### PW85\_DIM

The dimension of the physical space (3).

### PW85\_SYM

The dimension of the space of symmetric matrices (6).

### PW85\_LAMBDA\_ATOL

The absolute tolerance for the stopping criterion of Brent's method (in function [pw85\\_contact\\_function\(\)](#)).

### PW85\_MAX\_ITER

The maximum number of iterations of Brent's method (in function [pw85\\_contact\\_function\(\)](#)).

### PW85\_NR\_ITER

The total number of iterations of the Newton–Raphson refinement phase (in function [pw85\\_contact\\_function\(\)](#)).

void **pw85\_\_cholesky\_decomp**(double **const** *a*[PW85\_SYM], double *l*[PW85\_SYM])

Compute the Cholesky decomposition of a symmetric, positive matrix.

Let *A* be a symmetric, positive matrix, defined by the `double[6]` array *a*. This function computes the lower-triangular matrix *L*, defined by the `double[6]` array *l*, such that  $L^T \cdot L = A$ .

The array *l* must be pre-allocated; it is modified by this function. Note that storage of the coefficients of *L* is as follows:

$$L = \begin{bmatrix} l[0] & 0 & 0 \\ l[1] & l[3] & 0 \\ l[2] & l[4] & l[5] \end{bmatrix}.$$

void **pw85\_\_cholesky\_solve**(double **const** *l*[PW85\_SYM], double **const** *b*[PW85\_DIM], double *x*[PW85\_DIM])

Compute the solution to a previously Cholesky decoposed linear system.

Let *L* be a lower-triangular matrix, defined by the `double[6]` array *l* (see [pw85\\_\\_cholesky\\_decomp\(\)](#) for ordering of the coefficients). This function solves (by substitution) the linear system  $L^T \cdot L \cdot x = b$ , where the vectors *x* and *b* are specfied through their `double[3]` array of coordinates; *x* is modified by this function.

void **pw85\_\_residual**(double *lambda*, double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double *out*[3])

Compute the residual  $g(\lambda) = \mu_2^2 - \mu_1^2$ .

See [Optimization of the function \*f\*](#) for the definition of *g*. The value of  $\lambda$  is specified through the parameter *lambda*. See [pw85\\_contact\\_function\(\)](#) for the definition of the parameters *r12*, *q1* and *q2*.

The preallocated `double[3]` array *out* is updated with the values of  $f(\lambda)$ ,  $g(\lambda)$  and  $g'(\lambda)$ :

$$\text{out}[0] = f(\lambda), \quad \text{out}[1] = g(\lambda) \quad \text{and} \quad \text{out}[2] = g'(\lambda).$$

This function is used in function `pw85_contact_function()` for the final Newton–Raphson refinement step.

void **pw85\_spheroid**(double *a*, double *c*, double *n*[PW85\_DIM], double *q*[PW85\_SYM])

Compute the quadratic form associated to a spheroid.

The spheroid is defined by its equatorial radius *a*, its polar radius *c* and the direction of its axis of revolution, *n*.

*q* is the representation of a symmetric matrix as a double[6] array. It is modified in-place.

double **pw85\_f\_neg**(double *lambda*, double **const** \**params*)

Return the value of the opposite of the function *f* defined as (see [Theory](#)):

$$f(\lambda) = \lambda(1-\lambda) r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2,$$

where ellipsoids 1 and 2 are defined as the sets of points *m* (column-vector) such that:

$$(m - c_i) \cdot Q_i^{-1} \cdot (m - c_i) \leq 1$$

In the above inequality, *c<sub>i</sub>* is the center; *r<sub>12</sub>* = *c<sub>2</sub>* - *c<sub>1</sub>* is the center-to-center radius-vector, represented by the first 3 coefficients of the array *params*. The symmetric, positive-definite matrices *Q<sub>1</sub>* and *Q<sub>2</sub>* are specified through the next 12 coefficients. In other words, if *r12*, *Q1* and *Q2* were defined as usual by their double[3], double[6] and double[6] arrays *r12*, *q1* and *q2*, then *params* would be formed as follows:

```
double params[] = {r12[0], r12[1], r12[2],
                  q1[0], q1[1], q1[2], q1[3], q1[4], q1[5],
                  q2[0], q2[1], q2[2], q2[3], q2[4], q2[5]};
```

The value of *λ* is specified through the parameter *lambda*.

This function returns the value of  $-f(\lambda)$  (the “minus” sign comes from the fact that we seek the maximum of *f*, or the minimum of  $-f$ ).

This implementation uses [Cholesky decompositions](#). Its somewhat awkward signature is defined in accordance with `gsl_min.h` from the GNU Scientific Library.

int **pw85\_contact\_function**(double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double *out*[2])

Compute the value of the contact function of two ellipsoids.

The center-to-center radius-vector is specified by the double[3] array *r12*. The symmetric, positive-definite matrices *Q<sub>1</sub>* and *Q<sub>2</sub>* that define the two ellipsoids are specified through the double[6] arrays *q1* and *q2*.

This function returns the value of  $\mu^2$ , defined as (see [Theory](#)):

$$\mu^2 = \max\{ \lambda(1-\lambda) r_{12}^T \cdot [(1-\lambda)Q_1 + \lambda Q_2]^{-1} \cdot r_{12}, \quad 0 \leq \lambda \leq 1 \},$$

and the maximizer *λ*. Both values are stored in the preallocated double[2] array *out*:

$$\text{out}[0] = \mu^2 \quad \text{and} \quad \text{out}[1] = \lambda.$$

*μ* is the common factor by which the two ellipsoids must be scaled (their centers being fixed) in order to be tangentially in contact.

This function returns 0

---

**Todo:** This function should return an error code.

---

## 8.3 The “legacy” API

The functions described below belong to the legacy API. These are functions that have been superseded by equivalent (more accurate or more efficient) implementations in the core library. To use these functions in your code, you must include the following header:

```
#include <pw85_legacy.h>
```

and use the following link directive:

```
-lpw85_legacy
```

double **pw85\_legacy\_\_det\_sym**(double *a*[PW85\_SYM])

Return the determinant of *A*.

The symmetric matrix *A* is specified through the double[6] array *a*.

double **pw85\_legacy\_\_xT\_adjA\_x**(double *x*[PW85\_DIM], double *a*[PW85\_SYM])

Return the product  $x^T \cdot \text{adj}(A) \cdot x$ .

The column vector *x* is specified as a double[3] array. The symmetric matrix *A* is specified through the double[6] array *a*.

$\text{adj}(A)$  denotes the adjugate matrix of *A* (transpose of its cofactor matrix), see e.g. [Wikipedia](#).

void **pw85\_legacy\_\_detQ\_as\_poly**(double *q1*[PW85\_SYM], double *q2*[PW85\_SYM], double *q3*[PW85\_SYM], double *q4*[PW85\_SYM], double *b*[PW85\_DIM + 1])

Compute the coefficients of the polynomial  $\lambda \mapsto \det[(1-\lambda)Q_1 + \lambda Q_2]$ .

The symmetric, positive definite, 3×3 matrices *Q*<sub>1</sub> and *Q*<sub>2</sub> are specified as arrays *q1* and *q2*. The arrays *q3* and *q4* must hold the difference 2*Q*<sub>1</sub> - *Q*<sub>2</sub> and average (*Q*<sub>1</sub> + *Q*<sub>2</sub>)/2, respectively:

```
q3[i] = 2*q1[i] - q2[i] and q4[i] = 0.5*(q1[i] + q2[i]),
```

for *i* = 0, ..., PW85\_SYM-1. The returned polynomial has degree PW85\_DIM:

```
det[(1-λ)Q1+λQ2] = b0 + b1λ + b2λ2 + b3λ3.
```

The coefficients *b*<sub>*i*</sub> are stored in *b* in *increasing* order: *b*[*i*] = *b*<sub>*i*</sub>.

double **pw85\_\_rT\_adjQ\_r\_as\_poly**(double *r*[PW85\_DIM], double *q1*[PW85\_SYM], double *q2*[PW85\_SYM], double *q3*[PW85\_SYM], double *a*[PW85\_DIM])

Compute the coefficients of the polynomial  $\lambda \mapsto r^T \cdot \text{adj}[(1-\lambda)Q_1 + \lambda Q_2] \cdot r$ .

The symmetric, positive definite, 3×3 matrices *Q*<sub>1</sub> and *Q*<sub>2</sub> are specified as arrays *q1* and *q2*. The array *q3* must hold the difference 2*Q*<sub>1</sub> - *Q*<sub>2</sub>:

```
q3[i] = 2*q1[i] - q2[i],
```

for *i* = 0, ..., PW85\_SYM-1. The returned polynomial has degree PW85\_DIM - 1:

$$r^T \cdot \text{adj}[(1-\lambda)Q_1 + \lambda Q_2] \cdot r = a_0 + a_1 \lambda + a_2 \lambda^2.$$

The coefficients  $a_i$  are stored in  $a$  in *increasing* order:  $a[i] = a_i$ .

double **pw85\_legacy\_f1**(double *lambda*, double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double \**out*)

Return the value of the function  $f$  defined as (see [Theory](#)):

$$f(\lambda) = \lambda(1-\lambda) r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2,$$

where ellipsoids 1 and 2 are defined as the sets of points  $m$  (column-vector) such that:

$$(m - c_i) \cdot Q_i^{-1} \cdot (m - c_i) \leq 1$$

In the above inequality,  $c_i$  is the center;  $r_{12} = c_2 - c_1$  is the center-to-center radius-vector, represented by the double[3] array *r12*. The symmetric, positive-definite matrices  $Q_1$  and  $Q_2$  are specified through the double[6] arrays *q1* and *q2*.

The value of  $\lambda$  is specified through the parameter *lambda*.

This function returns the value of  $f(\lambda)$ . If *out* is not NULL, then it must be a pre-allocated double[3] array which is updated with the values of the first and second derivatives:

$$\text{out}[0] = f(\lambda), \quad \text{out}[1] = f'(\lambda) \quad \text{and} \quad \text{out}[2] = f''(\lambda).$$

This implementation uses [Cholesky decompositions](#).

double **pw85\_legacy\_f2**(double *lambda*, double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double \**out*)

Alternative implementation of [pw85\\_legacy\\_f1\(\)](#).

See [pw85\\_legacy\\_f1\(\)](#) for the meaning of the parameters *lambda*, *r12*, *q1* and *q2*.

This function returns the value of  $f(\lambda)$ . If *out* is not NULL, then it must be a pre-allocated double[1] array which is updated with the value of  $f(\lambda)$ .

This implementation uses [rational fractions](#).

---

**Todo:** This function should also compute the first and second derivatives.

---

int **pw85\_legacy\_contact\_function1**(double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double *out*[2])

Compute the value of the contact function of two ellipsoids.

See [pw85\\_contact\\_function\(\)](#) for the invocation of this function.

Implementation of this function relies on Newton–Raphson iterations on  $f$ ; it is not robust.

This function returns 0

---

**Todo:** This function should return an error code.

---

int **pw85\_legacy\_contact\_function2**(double **const** *r12*[PW85\_DIM], double **const** *q1*[PW85\_SYM], double **const** *q2*[PW85\_SYM], double *out*[2])

Compute the value of the contact function of two ellipsoids.

See [\*pw85\\_contact\\_function\(\)\*](#) for the invocation of this function.

This implementation uses the representation of  $f$  as *rational fractions*. Finding the maximum of  $f$  is then equivalent to finding the root of the numerator of the rational fraction of  $f'$ . For the sake of robustness, bisection is used to compute this root.

This function returns 0

---

**Todo:** This function should return an error code.

---



## THE PYTHON API

**Contents**

- *The new API*
  - *Representation of vectors and matrices*
- *The “legacy” API*

## 9.1 The new API

Overlap test of two ellipsoids.

This module provides a wrapper around the PW85 C library that implements the “contact function” defined by Perram and Wertheim (J. Comp. Phys. 58(3), 409–416, DOI:10.1016/0021-9991(85)90171-8) for two ellipsoids. Given two ellipsoids, this function returns the *square* of the common factor by which both ellipsoids must be scaled (their centers being fixed) in order to be tangentially in contact.

This module is released under a BSD 3-Clause License.

### 9.1.1 Representation of vectors and matrices

An ellipsoid is defined from its center  $c$  (a  $3 \times 1$ , column-vector) and quadratic form  $Q$  (a  $3 \times 3$ , symmetric, positive definite matrix) as the set of points  $m$  such that:

$$(m - c)^T \cdot Q^{-1} \cdot (m - c) \leq 1.$$

In this module, objects referred to as “vectors” are length-3 arrays of `double` coordinates. In other words, the representation of the vector  $x$  is the `double[3]` array  $x$  such that:

$$x = \begin{bmatrix} x[0] \\ x[1] \\ x[2] \end{bmatrix}.$$

Objects referred to as “symmetric matrices” (or “quadratic forms”) are length-6 arrays of `double`. Such arrays list in row-major order the coefficients of the triangular upper part. In other words, the representation of a the symmetric matrix  $A$  is the array  $a$  such that:

$$A = \begin{bmatrix} a[0] & a[1] & a[2] \\ & a[3] & a[4] \\ \text{sym.} & & a[5] \end{bmatrix}.$$

The present wrapper around the PW85 C library relies on the NumPy library. “double[n] array” should be understood here as “NumPy array with shape == (n,) and dtype == numpy.float64.”

Note that true NumPy array *must* be passed (array-likes will *not* work).

`pw85._cholesky_decomp(a, l=None)`

Compute the Cholesky decomposition  $A = L \cdot L^T$  of a 3×3 matrix.

A is a symmetric matrix, L is a lower matrix, both represented by double[6] arrays.

This function returns l, suitably updated with the coefficients of the Cholesky decomposition. If l is None, then a new array is allocated.

`pw85._cholesky_solve(l, b, x=None)`

Compute the solution of the 3×3 linear system  $L \cdot L^T \cdot x = b$ .

L is a lower matrix, represented by the double[6] array l; x and b are vectors (double[3] arrays).

This function returns x, suitably updated with the solution to the system. If x is None, then a new array is allocated.

`pw85.contact_function(r12, q1, q2, out=None)`

Return the value of the contact function of two ellipsoids.

See [f\(\)](#) for the meaning of the parameters r12, q1 and q2.

This function returns the pair  $(\mu^2, \lambda)$ , defined as (see [Theory](#)):

$$\mu^2 = \max\{ \lambda(1-\lambda)r_{12}^T \cdot [(1-\lambda)Q_1 + \lambda Q_2]^{-1} \cdot r_{12}, \ 0 \leq \lambda \leq 1 \}$$

(the returned value of  $\lambda$  is the actual maximizer).

$\mu$  is the common factor by which the two ellipsoids must be scaled (their centers being fixed) in order to be tangentially in contact.

If out is not None, it must be a pre-allocated double[2] array. It is updated with the values of  $\mu^2$ , and the maximizer  $\lambda$ :

$$\text{out}[0] = \mu^2 \quad \text{and} \quad \text{out}[1] = \lambda.$$

`pw85.f(lambda_, r12, q1, q2)`

Return the value of the function f defined as:

$$f(\lambda) = \lambda(1-\lambda)r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2,$$

where ellipsoids 1 and 2 are defined as the sets of points m (column-vector) such that:

$$(m - c_i) \cdot Q_i^{-1} \cdot (m - c_i) \leq 1$$

In the above inequality,  $c_i$  is the center;  $r_{12} = c_2 - c_1$  is the center-to-center radius-vector, represented by the double[3] array r12. The symmetric, positive-definite matrices  $Q_1$  and  $Q_2$  are specified through the double[6] arrays q1 and q2.

The value of  $\lambda$  is specified through the parameter lambda\_.

This function returns the value of  $f(\lambda)$ .

`pw85.spheroid(a, c, n, q=None)`

Return the quadratic form associated to a spheroid.

The spheroid is defined by its equatorial radius  $a$ , its polar radius  $c$  and the direction of its axis of revolution,  $n$  (vector, a.k.a. `double[3]` array).

If  $q$  is not `None`, then it must be a pre-allocated `double[6]` array. It is modified in place.

## 9.2 The “legacy” API

Python wrapper to the legacy API of PW85.

This module offers some implementations of the function  $f$  that were eventually discarded (for accuracy reasons). These functions are kept for reference.

The present wrapper around the legacy PW85 C library relies on the NumPy library. “`double[n]` array” should be understood here as “NumPy array with `shape == (n,)` and `dtype == numpy.float64`.”

Note that true NumPy array *must* be passed (array-likes will *not* work).

`pw85.legacy._detQ_as_poly(q1, q2, q3=None, q4=None, b=None)`

Compute the coefficients of the polynomial  $\lambda \mapsto \det[(1-\lambda)Q_1 + \lambda Q_2]$ .

The symmetric, positive definite,  $3 \times 3$  matrices  $Q_1$  and  $Q_2$  are specified as arrays `q1` and `q2`. If  $q3$  is not `None`, it must hold the difference  $2Q_1 - Q_2$ ; if  $q4$  is not `None`, it must hold the average  $(Q_1 + Q_2)/2$ :

```
q3[i] = 2*q1[i] - q2[i] and q4[i] = 0.5*(q1[i] + q2[i]),
```

for  $i = 0, \dots, 5$ . The returned polynomial has degree 3:

```
det[(1-λ)Q1+λQ2] = b0 + b1λ + b2λ2 + b3λ3.
```

If  $b$  is not `None`, it must be a pre-allocated `double[4]` array. It is modified in place with the coefficients  $b_i$ , stored in *increasing* order:  $b[i] = b_i$ .

If  $b$  is `None`, a new `double[4]` array is created and returned.

`pw85.legacy._det_sym(a)`

Return the determinant of  $A$ .

The symmetric matrix  $A$  is specified through the `double[6]` array  $a$ .

`pw85.legacy._rT_adjQ_r_as_poly(r, q1, q2, q3=None, a=None)`

Compute the coefficients of the polynomial  $\lambda \mapsto r^T \cdot \text{adj}[(1-\lambda)Q_1 + \lambda Q_2] \cdot r$ .

The symmetric, positive definite,  $3 \times 3$  matrices  $Q_1$  and  $Q_2$  are specified as arrays `q1` and `q2`. If  $q3$  is not `None`, it must hold the difference  $2Q_1 - Q_2$ :

```
q3[i] = 2*q1[i] - q2[i],
```

for  $i = 0, \dots, 5$ . The returned polynomial has degree 2:

```
rT·adj[(1-λ)Q1+λQ2]·r = a0 + a1λ + a2λ2.
```

If  $a$  is not `None`, it must be a pre-allocated `double[3]` array. It is modified in place with the coefficients  $a_i$ , stored in *a* in *increasing* order:  $a[i] = a_i$ . The function returns  $a$ .

If  $a$  is `None`, a new `double[3]` array is created and returned.

`pw85.legacy._xT_adjA_x(x, a)`

Return the product  $x^T \cdot \text{adj}(A) \cdot x$ .

The column vector  $x$  is specified as a `double[3]` array. The symmetric matrix  $A$  is specified through the `double[6]` array  $a$ .

$\text{adj}(A)$  denotes the adjugate matrix of  $A$  (transpose of its cofactor matrix), see e.g. [Wikipedia](#).

`pw85.legacy.f1(lambda_, r12, q1, q2, out=None)`

Return the value of the function  $f$  defined as (see [Theory](#)):

$$f(\lambda) = \lambda(1-\lambda) r_{12}^T \cdot Q^{-1} \cdot r_{12},$$

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2,$$

where ellipsoids 1 and 2 are defined as the sets of points  $m$  (column-vector) such that:

$$(m - c_i) \cdot Q_i^{-1} \cdot (m - c_i) \leq 1$$

In the above inequality,  $c_i$  is the center;  $r_{12} = c_2 - c_1$  is the center-to-center radius-vector, represented by the `double[3]` array `r12`. The symmetric, positive-definite matrices  $Q_1$  and  $Q_2$  are specified through the `double[6]` arrays `q1` and `q2`.

The value of  $\lambda$  is specified through the parameter `lambda_`.

This function returns the value of  $f(\lambda)$ . If `out` is not `None`, then it must be a pre-allocated `double[3]` array which is updated with the values of the first and second derivatives:

$$\text{out}[0] = f(\lambda), \quad \text{out}[1] = f'(\lambda) \quad \text{and} \quad \text{out}[2] = f''(\lambda).$$

This implementation uses [Cholesky decompositions](#).

`pw85.legacy.f2(lambda_, r12, q1, q2, out=None)`

Alternative implementation of [f1\(\)](#).

See [f1\(\)](#) for the meaning of the parameters `lambda_`, `r12`, `q1` and `q2`.

This function returns the value of  $f(\lambda)$ . If `out` is not `None`, then it must be a pre-allocated `double[1]` array which is updated with the value of  $f(\lambda)$ .

This implementation uses [rational fractions](#).

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