Documentation of the pw85 library

Release 2.0

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CONTENTS

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.

CHAPTER

ONE

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 3×1 column-vector of their coordinates in a global cartesian frame. For $i = 1, 2$, $E_i \subset \mathbb{R}^3$ denotes the following ellipsoid:

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

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:

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

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 $(0, 1)$:

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

It turns out that the contact function has a simple geometric interpretation. Indeed, μ 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 Φ is small. Indeed, let us consider a pair of ellipsoids (E_1, E_2) for which the true value of Φ, $\Phi_e(E_1, E_2)$, is close to the machine epsilon. Then, the numerical estimate of Φ, $\Phi_e(E_1, E_2)$, 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 $E_1, \ldots, E_n$ do overlap, a simulated annealing strategy is adopted to minimize the quantity $U(E_1, \ldots, E_n)$ defined as follows:

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

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 sentense 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 boost::mathGNU (for its implementation of the Brent algorithm).

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 pybind11) 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 `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 λ is found such that `f > 1`, then μ^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 (see Issue XXX).
3. …

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`.

CHAPTER

TWO

INSTALLATION

Contents

First of all, clone the repository

```
$ git clone https://github.com/sbrisard/pw85
```

2.1 Installing the C++ library

pw85 is a header-only library: there is no installation procedure *per se* and you can drop the header wherever you like (as long as it is located in a `pw85` subdirectory). To use pw85 in a C++ project, you must include the header

```
#include <pw85/pw85.hpp>
```

and inform the compiler of its location.

Note: pw85 depends on Boost::Math (for the implementation of the Brent algorithm). You must pass the relevant options to the compiler. Typically, these would be `-I` options. The C++ tutorials provides a *CMake example*.

To run the tests or build the documentation properly, you need to first build the python bindings (see *below*).

To further test your installation, build the example in the *C++ tutorial*.

2.2 Installing the Python bindings

The Python bindings are built with pybind11, which must be installed.

To install the pw85 module, `cd` into the `python` subdirectory and run the `setup.py` script as follows.

First, build the extension:

```
$ python setup.py build_ext -Ipath/to/boost/math
```

When the extension is built, installation is down as usual:

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

or (if you intend to edit the project):

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

To run the tests with Pytest:

```
$ python -m pytest tests
```

(beware, these tests take some time!).

2.3 Building the documentation

Note: For the documentation to build properly, the python module must be installed, as it is imported to retrieve the project metadata.

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 `docs` subdirectory:

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

To build the LaTeX version of the docs:

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

CHAPTER

THREE

TUTORIAL

Contents

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

Ellipsoid E_1 is an oblate spheroid centered at point `x1 = (-0.5, 0.4, -0.7)`, with equatorial radius `a1 = 10`, polar radius `c1 = 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 `a1 = 0.5`, polar radius `c1 = 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. Note that these arrays must be *preallocated*:

```
>>> q1 = np.empty((6,), dtype=np.float64)
>>> pw85.spheroid(a1, c1, n1, q1)
>>> q1
array([ 1.e+02, -0.e+00, -0.e+00,  1.e+02, -0.e+00,  1.e-02])
>>> q2 = np.empty_like(q1)
>>> pw85.spheroid(a2, c2, n2, q2)
>>> 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()`:

```
>>> out = np.empty((2,), dtype=np.float64)
>>> pw85.contact_function(r12, q1, q2, out)
>>> mu2, lambda_ = out
>>> 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.))
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 corectness of the value found for the scaling factor μ. 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 λ 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 ellispoid E_i is scaled by μ, then its matrix representation

Q_i is scaled by μ^2, and its inverse Q_i^{-1} is scaled by μ^{-2}.

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

```
>>> x = x0-x1
>>> Q1_inv.dot(x).dot(x)
1.0000000000058238
```

```
>>> x = x0-x2
>>> Q2_inv.dot(x).dot(x)
0.9999999999988334
```

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 undelying C++ API. The following C++ program (`download source file`) defines the two ellipsoids, then computes μ^2 and λ:

```
#include <iostream>
#include <array>

#include "pw85/pw85.hpp"

using Vec = std::array<double, pw85::dim>;
using SymMat = std::array<double, pw85::sym>;

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

  Vec x2{0.2, -0.3, 0.4};
```

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```
  Vec n2{1., 0., 0.};
  double a2 = 0.5;
  double c2 = 5.;

  Vec r12;
  for (int i = 0; i < pw85::dim; i++) r12[i] = x2[i] - x1[i];

  SymMat q1, q2;
  pw85::spheroid(a1, c1, n1.data(), q1.data());
  pw85::spheroid(a2, c2, n2.data(), q2.data());

  std::array<double, 2> out;
  pw85::contact_function(r12.data(), q1.data(), q2.data(), out.data());
  std::cout << "mu^2 = " <<  out[0] << std::endl;
  std::cout << "lambda = " << out[1] << std::endl;
}
```

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

```
cmake_minimum_required(VERSION 3.13)

project("tutorial" LANGUAGES CXX)
set(CMAKE_CXX_STANDARD 17)

add_executable(${PROJECT_NAME} ${PROJECT_NAME}.cpp)

find_library(MATH_LIBRARY m)
if (MATH_LIBRARY)
    target_link_libraries(${PROJECT_NAME} INTERFACE ${MATH_LIBRARY})
endif()

find_package(Boost REQUIRED)
target_link_libraries(${PROJECT_NAME} PRIVATE Boost::headers)

target_include_directories(${PROJECT_NAME} PRIVATE "../../include")
```

`cd` into the `cpp_tutorial` subdirectory. The provided example program should be compiled and linked against pw85:

```
$ mkdir build
$ cd build
$ cmake ..
$ 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
```

CHAPTER

FOUR

THEORY

Contents

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 3×1 column-vector of its coordinates. Likewise, a second-rank tensor is represented by its 3×3 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:

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

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

$$Q = \sum_i a_i^2 \, v_i \cdot v_i^{\mathsf{T}}, \tag{2}$$

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:

$$Q = \begin{pmatrix} q[0] & q[1] & q[2] \\ & q[3] & q[4] \\ \text{sym.} & & q[5] \end{pmatrix}. \tag{3}$$

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

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

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

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

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:

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

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

$$\nabla F(x_0(\lambda), \lambda) = 0, \tag{7}$$

which leads to:

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

and can be rearranged:

$$x_0(\lambda) - c_1 = (1-\lambda) Q_1 \cdot Q^{-1} \cdot r_{12}, \tag{9a}$$
$$x_0(\lambda) - c_2 = -\lambda Q_2 \cdot Q^{-1} \cdot r_{12}, \tag{9b}$$

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2. \tag{10}$$

It results from the above that:

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

Maximization of f with respect to λ now delivers the stationarity condition:

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

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 μ^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, μ^2 is the value of the contact function.

We are now in a position to give a geometric interpretation of μ. It results from Eq. *(13)* and the definition of μ 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 μ.

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

CHAPTER

FIVE

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 λ to equation $f'(\lambda) = 0$, where it is recalled that f is defined as follows:

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

with:

$$Q = (1-\lambda)Q_1 + \lambda Q_2. \tag{2}$$

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:

$$Q = L\cdot L^{T}, \tag{3}$$

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:

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

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:

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

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

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

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

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

and:

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

Therefore:

```
(9)    f″(λ) = -2rᵀ·s - 2(1-2λ)sᵀ·u + 2λ(1-λ)uᵀ·v.
```

5.2 Implementation #2: using rational functions

We observe that `f(λ)` is a rational function [see Eq. *(1)*], and we write:

```
                λ(1-λ)a(λ)
(10)    f(λ) = ──────────,
                  b(λ)
```

with:

```
(11a)    a(λ) = r₁₂ᵀ·adj[(1-λ)Q₁+λQ₂]·r₁₂ = a₀ + a₁λ + a₂λ²,

(11b)    b(λ) = det[(1-λ)Q₁+λQ₂] = b₀ + b₁λ + b₂λ² + b₃λ³,
```

where `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(λ)` and `b(λ)` for specific values of `λ`:

```
(12a)    a₀ = a(0),

               a(1) - a(-1)
(12b)    a₁ = ────────────,
                    2

               a(1) + a(-1)
(12c)    a₂ = ──────────── - a(0),
                    2

(12d)    b₀ = b(0),

               8b(½)             b(1)   b(-1)
(12e)    b₁ = ─────  - 2b(0) - ──── - ─────
                 3                2      6

               b(1) + b(-1)
(12f)    b₂ = ──────────── - b(0),
                    2

                8b(½)                    b(-1)
(12g)    b₃ = -─────  + 2b(0) + b(1) - ─────.
                  3                       3
```

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

Evaluating the derivative of `f` with respect to `λ` 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:

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

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

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

with:

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

Solving $f'(\lambda) = 0$ for λ 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 λ is found, μ 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 (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_radii;
  double *radii;
  read_dataset_double(hid, "/radii", &num_radii, &radii);

  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`.

Note: The provided script refers to an old implementation of pw85.

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.

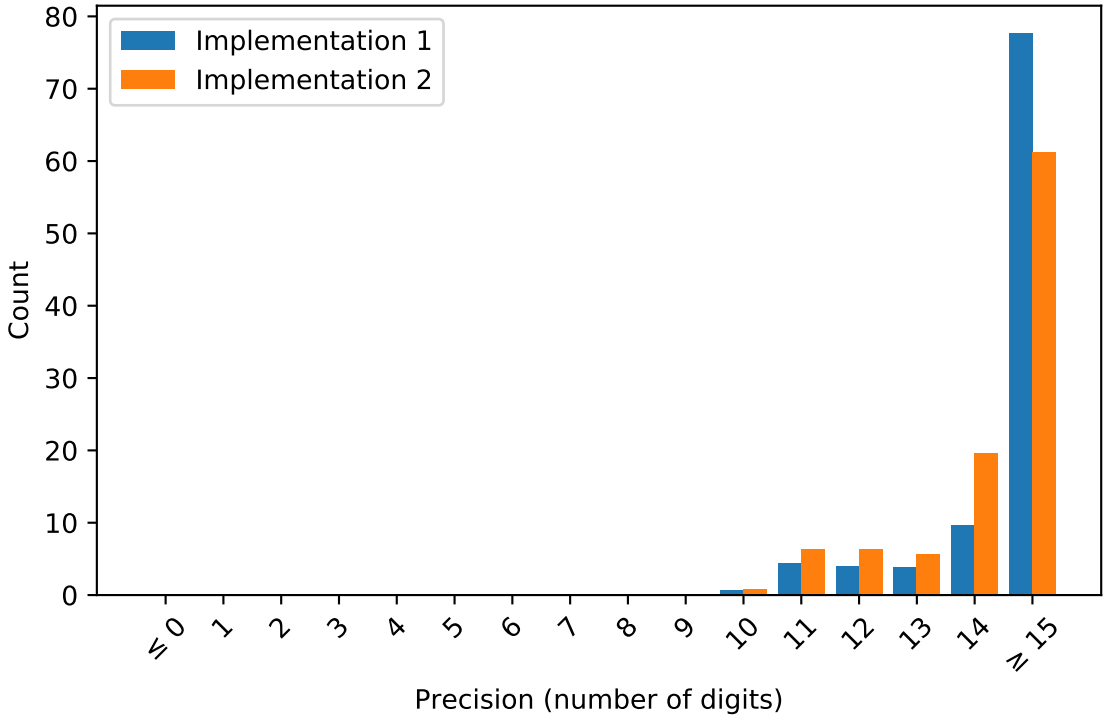

Fig. 5.1: Accuracy of the two implementations.

CHAPTER

SIX

OPTIMIZATION OF THE FUNCTION f

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

Given that the first and second derivatives of f can be computed explicitely (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 otpimization 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 Boost::Math library. However, this method delivers a relatively low accuracy of the maxmimizer 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 λ we can define two values of μ^2: one is provided by Eq. *(9a)*, the other one is given by Eq. *(9b)* (both in chapter *Theory*):

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

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

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

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

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

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 λ such that $\mu_1^2 = \mu_2^2$. We therefore define the following residual:

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

and we need to find λ 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:

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

Eqs. *(4)* and *(5)* are then used for the final, refinement step of determination of λ.

CHAPTER

SEVEN

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 sheroids, 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 λ and μ^2.

We first assert that μ_1^2 and μ_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 λ for the stopping criterion of the Brent iterations, as defined by the constant *pw85::lambda_atol*.

CHAPTER

EIGHT

THE C++ API

Note: functions whose name is prefixed with an underscore should be considered as "private": these functions are exposed for testing purposes. They 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 3×1, column-vector) and quadratic form `Q` (a 3×3, 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 API

namespace **pw85**

Functions

void **_cholesky_decomp**(double const *a, double *l)
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`$^{\intercal}$`·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[0]    0    0 ⎤
L = ⎢ l[1] l[3]    0 ⎥.
    ⎣ l[2] l[4] l[5] ⎦
```

void **_cholesky_solve**(const double *l, const double *b, double *x)
Compute the solution to a previously Cholesky decomposed 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`$^{\intercal}$`·L·x = b`, where the vectors `x` and `b` are specified through their `double[3]` array of coordinates; `x` is modified by this function.

void **spheroid**(double a, double c, const double *n, double *q)
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` (unit-vector, `double[3]` array).

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

double **f_neg**(double lambda, const double *r12, const double *q1, const double *q2)
Return the value of the opposite of the function `f` defined as (see *Theory*).

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

with

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

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

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

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 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**.

void **_residual**(double lambda, const double *r12, const double *q1, const double *q2, double *out)
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 λ is specified through the parameter `lambda`. See *contact_function()* for the definition of the parameters `r12`, `q1` and `q2`.

The preallocated `double[3]` array `out` is updated as follows: `out[0]=` $f(\lambda)$, `out[1]=` $g(\lambda)$ and `out[2]=` $g'(\lambda)$.

This function is used in function *pw85::contact_function()* for the final Newton–Raphson refinement step.

int **contact_function**(const double *r12, const double *q1, const double *q2, double *out)
Compute the value of the contact function of two ellipsoids.

The center-to-center radius-vector r_{12} is specified by the `double[3]` array `r12`. The symmetric, positive-definite matrices Q_1 and Q_2 that define the two ellipsoids are specified through the `double[6]` arrays `q1` and `q2`.

This function computes the value of μ^2, defined as

$$\mu^2 = \max_{0 \le \lambda \le 1} \left\{ \lambda(1-\lambda) r_{12}^{\mathsf{T}} \cdot \left[(1-\lambda) Q_1 + \lambda Q_2 \right]^{-1} \cdot r_{12} \right\},$$

and the maximizer λ, see *Theory* . Both values are stored in the preallocated `double[2]` array `out`: `out[0]` = μ^2 and `out[1]` = λ.

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.

Variables

constexpr size_t **dim** = 3
The dimension of the physical space (3).

constexpr size_t **sym** = 6
The dimension of the space of symmetric matrices (6).

constexpr double **lambda_atol** = 1e-6
The absolute tolerance for the stopping criterion of Brent's method (in function *contact_function()*).

constexpr size_t **max_iter** = 25
The maximum number of iterations of Brent's method (in function *contact_function()*).

constexpr size_t **nr_iter** = 3
The total number of iterations of the Newton–Raphson refinement phase (in function *contact_function()*).

namespace **metadata**

Variables

constexpr std::string_view **author** = {"S. Brisard"}

constexpr std::string_view **description** = {"Implementation of 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."}

constexpr std::string_view **author_email** = {"sebastien.brisard@univ-eiffel.fr"}

constexpr std::string_view **license** = {"BSD 3-Clause License"}

constexpr std::string_view **name** = {"pw85"}

constexpr std::string_view **url** = {"https://github.com/sbrisard/pw85"}

constexpr std::string_view **version** = {"2.0"}

constexpr std::string_view **year** = {"2021"}

CHAPTER

NINE

THE PYTHON API

pypw85.**_cholesky_decomp**(*a: numpy.ndarray[numpy.float64], l: numpy.ndarray[numpy.float64]*) → None

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 `Lᵀ·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[0]    0    0 ⎤
L = ⎢ l[1] l[3]    0 ⎥.
    ⎣ l[2] l[4] l[5] ⎦
```

This function is exposed for testing purposes only.

pypw85.**_cholesky_solve**(*l: numpy.ndarray[numpy.float64], b: numpy.ndarray[numpy.float64], x: numpy.ndarray[numpy.float64]*) → None

Compute the solution to a previously Cholesky decomposed linear system.

Let `L` be a lower-triangular matrix, defined by the `double[6]` array `l` (see *_cholesky_decomp()* for ordering of the coefficients). This function solves (by substitution) the linear system `Lᵀ·L·x = b`, where the vectors `x` and `b` are specified through their `double[3]` array of coordinates; `x` is modified by this function.

This function is exposed for testing purposes only.

pypw85.**contact_function**(*r12: numpy.ndarray[numpy.float64], q1: numpy.ndarray[numpy.float64], q2: numpy.ndarray[numpy.float64], out: numpy.ndarray[numpy.float64]*) → int

Compute the value of the contact function of two ellipsoids.

See *f_neg()* for the meaning of the parameters *r12*, *q1* and *q2*.

This function computes the value of μ^2, defined as:

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

and the maximizer λ, see *Theory*. Both values are stored in the preallocated `double[2]` array `out`: `out[0]` = μ^2 and `out[1]` = λ.

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.

pypw85.**f_neg**(*lambda: float*, *r12: numpy.ndarray[numpy.float64]*, *q1: numpy.ndarray[numpy.float64]*, *q2: numpy.ndarray[numpy.float64]*) → float

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:

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

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 λ is specified through the parameter `lambda`.

This function returns the value of `-f(λ)` (the "minus" sign comes from the fact that we seek the maximum of `f`, or the minimum of `(-f)`.

This implementation uses *Cholesky decompositions*.

pypw85.**spheroid**(*a: float*, *c: float*, *n: numpy.ndarray[numpy.float64]*, *q: numpy.ndarray[numpy.float64]*) → None

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` (unit-vector, `double[3]` array).

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

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