

INRA
UR341 Mathématiques et informatique appliquées
Domaine de Vilvert
F-78350 Jouy-en-Josas

CaliFloPP

Version 2007-12-05

Calculation of the Integrated Flow of Particles between Polygons

Annie Bouvier, Kiên Kiêu, Katarzyna Adamczyk and Hervé Monod

September 21, 2009

Abstract

CaliFloPP is a software that calculates flows of particles between pairs of polygons, when given a so-called individual dispersal function. The individual dispersal function describes the particle dispersion between pairs of points, and **CaliFloPP** deduces the total flows between pairs of polygons. This integration problem is solved by reducing the dimension of the integral and by using algorithms from computational geometry.

The application implemented by default in **CaliFloPP** concerns gene flow between crop fields and their borders, through the dispersion of pollen and seed particles. More precisely, it allows an extension to very general field shapes of Genesys, a model and software on the population dynamics of cultivated and feral oilseed rape in an agricultural landscape ([CCDM01a] et [CCDM01b]).

This manual first describes the methods implemented in **CaliFloPP**. This is followed by installation, user and developer guides.

Résumé

Le programme **CaliFloPP** estime des flux de particules entre paires de polygones: à partir d'une fonction de dispersion dite individuelle, c'est-à-dire décrivant la dispersion des particules de point à point, il calcule les flux totaux émis d'un polygone à un autre. Ce problème d'intégration est résolu en réduisant la dimension de l'intégrale et en utilisant des algorithmes de géométrie algorithmique.

L'application implémentée dans le programme **CaliFloPP** est celle des flux de pollen et de graines de colza entre parcelles agricoles, à l'échelle d'une petite région. C'est une extension du modèle Genesys ([CCDM01a] et [CCDM01b]) de dynamique des populations cultivées et spontanées de colza entre les parcelles d'un paysage et leurs bordures, à la dispersion entre parcelles non quadrilatères.

Cette notice décrit les méthodes implémentées dans **CaliFloPP**. Elle inclut les guides d'installation, d'utilisation et de développement.

Credits

People in Charge

- Hervé Monod and Annie Bouvier, INRA, MIA, Jouy-en-Josas. <http://www.inra.fr/miaj>.

Authors

- Katarzyna Adamczyk, Annie Bouvier, Kiên Kiêu et Hervé Monod, INRA, MIA, Jouy-en-Josas. <http://www.inra.fr/miaj>
- Ying Fu developed the prototype: see [Y.05].

Other Participants

- Nathalie Colbach, INRA, UMR Biologie et Gestion des Adventices INRA-ENESAD-Université de Bourgogne, Dijon, wrote the seed dispersal function, improved the pollen dispersal function, tested the programme and gave advice for practical adjustments.
- Mathieu Leclaire, computer engineer of the European Project **SIGMEA** on gene flow modelling, tested the programme and gave advice for practical adjustments.

Contents

1	Introduction	9
1.1	Pollen and seed dispersal between fields	9
1.2	What CaliFloPP calculates : integrated flow of particles between polygons	9
1.3	What CaliFloPP can help to calculate : an example	10
1.4	The main steps of the CaliFloPP calculations	10
I	Methods for Particle Flow Integration	13
2	Integral Reduction	15
3	Geometric Computation	17
3.1	Area of a convex polygon	18
3.2	Intersection of two convex polygons	19
3.3	Minkowski sum of convex polygons	19
3.4	Convex partitioning of a polygon	21
4	Two-dimensional Numerical Integration	23
4.1	Smoothness of the integrand	23
4.2	Method based on grids of points	24
4.2.1	Additional results	25
4.3	Adaptive cubature method	25
II	Example	29
5	Example	31
5.1	Introduction	31
5.1.1	Data	31
5.2	Influence of the parameterisation in the grid method	31
5.2.1	Influence of the number of replications	31
5.2.2	Influence of the grid step	33
5.3	Influence of the parametrization in the cubature method	33
5.3.1	Influence of the number of evaluations	33
5.3.2	Influence of the required precision	34
5.4	Global comparison	34
5.4.1	Global summary	34
5.5	Influence of the dispersal function	37
5.6	Conclusion	37

III	Auxiliary packages	39
6	R Packages	41
6.1	Rcaliflopp	41
6.1.1	Example	41
6.2	landm	42
6.2.1	Example	42
IV	Installation Guide	45
7	Prerequisite	47
8	Installation Steps	49
9	Configuration	51
9.1	Input	52
9.2	Output	53
9.3	Error treatment	53
9.4	Landscape features	54
9.5	Individual dispersal functions	55
9.6	Methods features	55
9.6.1	Grid method	55
9.6.2	Cubature method	56
9.7	Numerical parameters	56
10	More options	57
V	User Guide	59
11	Quick Start	61
12	Input	63
12.1	The polygons-file	63
12.1.1	Constraints on the polygons	63
12.1.2	Syntax of the polygons file	63
12.2	Parameter file in non-interactive mode	64
12.3	Dialogue in interactive mode	66
13	Output	69
13.1	Screen output	69
13.2	Result file	70
13.3	Error treatment	71
14	Example	73
14.1	Polygons file	73
14.2	Calculation by the cubature method	73
14.2.1	Parameter file	73
14.2.2	Command line	73
14.2.3	Screen output	74

14.2.4	Output on the result-file	74
14.3	Calculation by the grid method	74
14.3.1	Parameter file	74
14.3.2	Command line	75
14.3.3	Screen output	75
14.4	Comparison under R	75
15	Details about the programme	77
15.1	The main steps of the programme	77
15.1.1	Preprocessing on the polygons	77
15.1.2	Steps for each pair of convex polygons	77
15.1.3	Integration methods	78
15.1.4	Final results	78
15.2	The individual dispersal functions	78
15.2.1	Individual dispersal function of oilseed rape pollen	78
15.2.2	Individual dispersal function of oilseed rape seeds	79
15.2.3	How to modify or add individual dispersal functions	79
16	Auxiliary Programmes	81
16.1	Polygon area computation	81
16.2	Computation of the area of the intersection between two polygons	81
16.3	Polygons simplification	82
16.4	R functions	82
17	A Small Glossary	83
VI	Developer Guide	85
18	Implementation	87
18.1	Programme steps	87
18.1.1	The main programme and the two pilots	87
18.1.2	Preprocessing	87
18.1.3	Calculation steps	87
18.1.4	Calculation by the grid method	88
18.1.5	Calculation by the cubature method	89
18.2	Data structures	90
18.3	Functions list	91
19	How to Modify	93
VII	Bibliography	95

Chapter 1

Introduction

1.1 Pollen and seed dispersal between fields

The development of genetically modified (GM) plants has triggered much research to study how different types of agriculture can co-exist on a given landscape. In particular, several models have been developed and implemented to quantitatively describe and predict the risks of contamination of non-GM fields by GM fields, such as Genesys for oilseed rape [CCDM01a, CCDM01b].

A key stage in models such as Genesys consists in calculating the pollen and seed flow between two fields A and B . In Genesys, this calculation is performed by integrating a plant-to-plant (or individual) dispersal function ϕ over all emitting plants in A and all receiving plants in B , where ϕ is a function of the distance between the emitting and the receiving plants. The individual dispersal functions ϕ have been previously determined by specifically designed experiments (see *e.g.* [LKV⁺98]). In practice, because the plant density is high in a cultivated field, the integration is made continuously over A and B .

The calculation of field-to-field pollen and seed dispersals is a key stage not only for biological but also for numerical reasons. First, it is a non-trivial programming task. Relatively simple algorithms can be imagined for integrating the dispersal function over pairs of fields, but they may not be able to cope properly with the large diversity of field sizes and shapes which are met in actual agricultural landscapes. Second, the calculation requires a lot of computing time and so it imposes limits on the size of the landscapes one wants to study. The initial motivation for developing CaliFloPP was precisely to make the calculation of pollen and seed flow in Genesys more general and more efficient.

1.2 What CaliFloPP calculates : integrated flow of particles between polygons

Pollen and seed dispersal between fields is just an example of phenomena involving flows of particles between polygonal objects. Other examples include the flow of pathogen spores between fields in plant epidemiology, or the flow of polluting particles between sites in environmental applications.

CaliFloPP is a general programme, which makes it possible to calculate such global flows efficiently between pairs of polygons, by integration of an individual dispersal function. When running CaliFloPP, the basic entries that one needs to specify are :

- the coordinates of the vertices of each polygon ;

- the individual dispersal function ϕ .

In CaliFloPP, the polygons are considered as *continuous* and *homogeneous* sources of emission and continuous and homogeneous reception areas. The individual dispersal function ϕ between two points x and y in \mathbb{R}^2 is assumed to depend on $x_2 - x_1$ and $y_2 - y_1$, so that the argument of ϕ is a two-dimensional vector. As a special case, the dispersal may be isotropic so that $\phi(y - x)$ depends on $\sqrt{(y_1 - x_1)^2 + (y_2 - x_2)^2}$ only.

For each pair of polygons A and B , CaliFloPP calculates the integrated flow from A to B , that is

$$\mathcal{F}(A, B) = \int_A \int_B \phi(y - x) dy dx. \quad (1.1)$$

1.3 What CaliFloPP can help to calculate : an example

In many applications, the calculations performed by CaliFloPP will just represent an initial step, making time-consuming calculations once and for all before simulating a more complex space-and-time model.

Consider for example a landscape constituted of non-GM oilseed rape fields, GM oilseed rape fields, and other fields. Then the expected rate of contamination (due to pollen only, for simplicity) on a given non-GM field B can be defined as the proportion of pollen received by B which has been emitted by neighbouring GM fields. In the present context, this is equal to

$$c = \frac{\sum_{GM\ fields\ A} \mathcal{F}(A, B)}{\sum_{GM\ fields\ A} \mathcal{F}(A, B) + \sum_{non-GM\ fields\ A} \mathcal{F}(A, B)}. \quad (1.2)$$

Thus, calculating the expected rate of contamination for all non-GM fields requires to calculate $\mathcal{F}(A, B)$ for all pairs of fields with A an oilseed rape field and B a non-GM oilseed rape field. In Genesys, such calculations are performed over several years with different allocations of crops from one year to the next one. Thus, there is an interest in calculating $\mathcal{F}(A, B)$ over all pairs of fields once and for all.

Note that a more general form of equation (1.2) is

$$c = \frac{\sum_{GM\ fields\ A} \alpha_A \mathcal{F}(A, B)}{\sum_{GM\ fields\ A} \alpha_A \mathcal{F}(A, B) + \sum_{non-GM\ fields\ A} \alpha_A \mathcal{F}(A, B)},$$

where α_A denotes the quantity of pollen per squared meter emitted by field A and $\phi(y - x)$ must be interpreted as the *proportion* of particles emitted at point x that arrives at point y . As this example shows, the CaliFloPP calculations are perfectly compatible with models involving different levels of emission or reception between polygons.

1.4 The main steps of the CaliFloPP calculations

According to equation (1.1), the calculation of $\mathcal{A}(A, B)$ requires a four-dimensional integration, since A and B are both two-dimensional. When $\mathcal{A}(A, B)$ must be calculated for many pairs of polygons, this represents a heavy lot of computing time.

In fact, the first step in CaliFloPP consists in reducing the dimension of the integral from 4 to 2. This is done by taking profit of the invariance properties of the dispersal function (see Chapter 2).

The price to pay for the dimension reduction is the arrival of geometrical quantities in the reduced integral, whose calculations are not trivial. These calculations, however, can be performed efficiently provided tools from *computational geometry* are used. This is explained in Chapter 3.

In order to apply some of these methods, it is necessary that the polygons be convex. Chapter 3.4 describes a method to partition any polygon into convex sub-polygons.

The second step consists in the integration *per se*, for which several approaches have been considered. Two of them have been implemented in CaliFloPP: one based on regular grids over the domain of integration, the other based on cubature integration methods. They are described in Chapter 4.

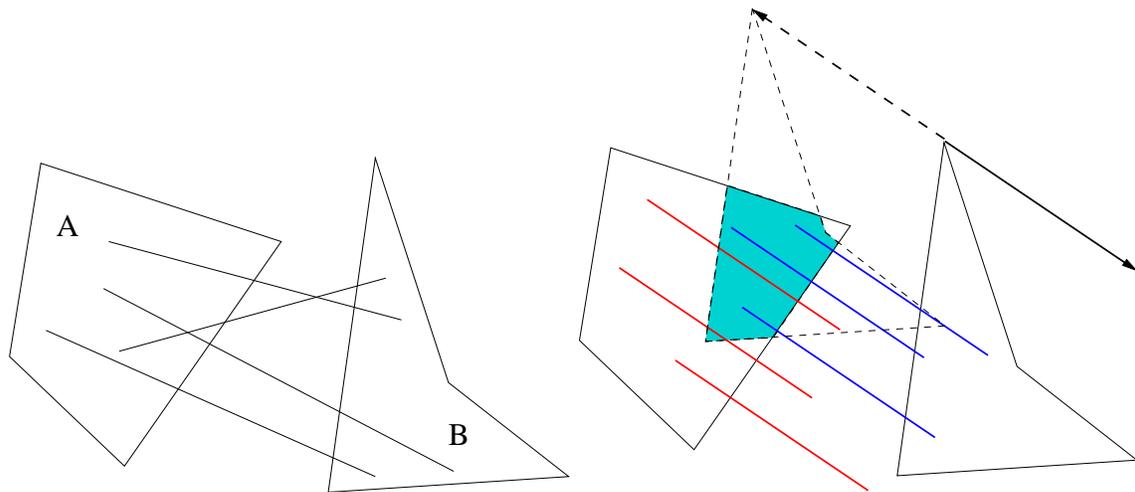
Part I

Methods for Particle Flow
Integration

Chapter 2

Integral Reduction

The quantity \mathcal{A} of particles from a polygon A to a polygon B , can be computed by integrating the individual dispersal function, $\phi(y - x)$, over pairs of points (x, y) , $x \in A$, $y \in B$, see Section 1 and Fig. 2.1.



(a) The first and second points of each pair can be chosen independently in A and B . (b) Consider all the pairs of points separated by the same vector t (t is in bold on the figure). For a given t , $x \in A$ and $x + t \in B$, if and only if $x \in A \cap (B - t)$ (such x and $x + t$ are joined here by blue segments; $A \cap (B - t)$ is represented by the blue area).

Figure 2.1: The quantity of particles from a polygon A to a polygon B is computed by integrating the individual dispersal function over all pairs of points $(x, y) \in A \times B$. These pairs are represented here by segments.

Rather than scrolling through the pairs of points by choosing each member independently in A and B , it is worth considering the pairs separated by the same vectors. The dispersal function is constant on such subsets of the pairs of points.

With the variable change $(x, y) \rightarrow (x, t = y - x)$, the set

$$\{y - x | x \in A, y \in B\}$$

can be written $\check{A} \oplus B$ where $\check{A} = -A$ and \oplus stands for the Minkowski sum. The Minkowski sum of two sets A and B is simply the set obtained by addition of the points of A and B (see Fig. 2.2). On the other hand, for each vector $t \in \check{A} \oplus B$:

$$x \in A, y = x + t \in B \Leftrightarrow x \in A \cap (B - t)$$

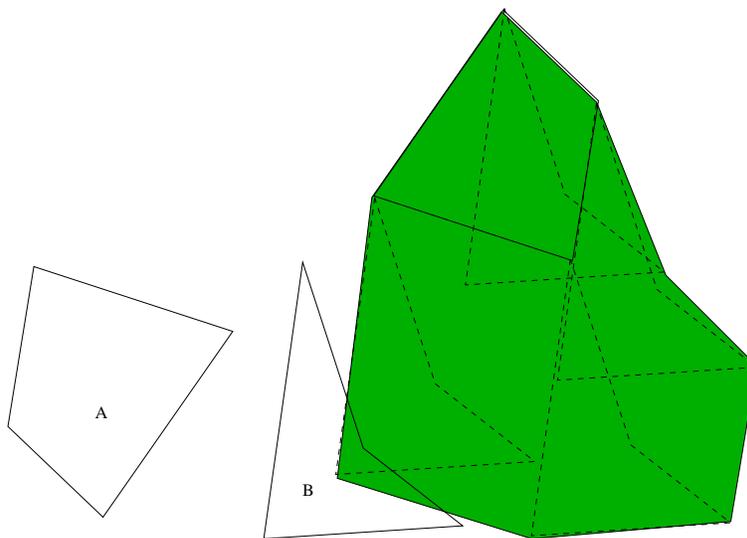


Figure 2.2: The set of points $t = y - x$, where $x \in A$ and $y \in B$, is written $\check{A} \oplus B$. It is the set of points covered by B when the vertex o is moved inside \check{A} . Here, to simplify, the origin of the plan o is located on a vertex of B .

Now, we can rewrite the integral \mathcal{F} defined by the equation (1.1):

$$\mathcal{F} = \int_{\check{A} \oplus B} \int_{A \cap (B-t)} \phi(t) dx dt \quad (2.1)$$

as:

$$\mathcal{F} = \int_{\check{A} \oplus B} \int_{A \cap (B-t)} dx \phi(t) dt. \quad (2.2)$$

The integral in x is simply the area of $A \cap (B - t)$, so:

$$\mathcal{F} = \int_{\check{A} \oplus B} \text{area}(A \cap (B - t)) \phi(t) dt \quad (2.3)$$

The computation of one of the two integrals has been replaced by the computation of an area and of an intersection, the intersection of A and a translation of B . The calculation of (2.3) has proven to be faster than the one of (1.1)¹ So, it is the formula implemented in CaliFloPP.

¹Time comparisons have been made by using the integration subroutines of the NAG [NAG] library, D01FCF (adaptive integration, i.e where the evaluation spots depend on the integrand), and D01GCG (Korobov-Conroy method) on real and simulated fields.

Chapter 3

Geometric Computation

In order to compute numerically the two-dimensional integral (2.3), one must compute the area of the intersection $\text{area}(A \cap (B - t))$ for different values of $t \in \check{A} \oplus B$ (domain of integration) where A and B are polygons. Note that A and B are not necessarily convex. Computations of polygonal areas, intersections and Minkowski sums are known problems in *computational geometry*. The textbook [O'R98] is a rather nice introduction to that topic. Most algorithms briefly described below are provided there. Note that this chapter is only devoted to the computation of the geometric features involved in the integral (2.3). The problem of numerical integration is treated in Chapter 4.

The intersection $A \cap (B - t)$ is a polygon. The computation of the area of a polygon is straightforward, see Section 3.1 for the case when the polygon is convex.

The computation of the intersection $A \cap (B - t)$ is easy when both A and B are convex, see Section 3.2. When either A or B is not convex, the intersection may be complicated. In particular, it may not be connected.

The computation of the Minkowski sum $\check{A} \oplus B$ is rather easy if A or B are convex, see Section 3.3.

Hence the computation of the integral (2.3) is easy when both A and B are convex. This is why we propose to first decompose A and B as unions of convex polygons:

$$A = \bigcup_{i=1}^n A_i, \quad B = \bigcup_{j=1}^m B_j, \quad (3.1)$$

where the areas of $A_i \cap A_{i'}$, respectively $B_j \cap B_{j'}$, are equal to 0 whenever $i \neq i'$, respectively $j \neq j'$. An algorithm for computing such a decomposition is described in Section 3.4. It is easy to check that the integral (2.3) can be written as:

$$\int_{\check{A} \oplus B} \text{area}(A \cap (B - t)) \phi(t) dt = \sum_{i=1}^n \sum_{j=1}^m \int_{\check{A}_i \oplus B_j} \text{area}(A_i \cap (B_j - t)) \phi(t) dt. \quad (3.2)$$

Based on the algorithm for decomposing polygons into convex ones and tools for computing numerically the integral (2.3) for any pair (A, B) of convex polygons (see Chapter 4), the integral (2.3) for an arbitrary pair of polygons can be computed using Algorithm 1.

Below, convex polygons are represented as sequences of vertices labeled counterclockwise: (v_0, \dots, v_{n-1}) . Many computations involve cycling over vertices. Hence it is convenient to use the convention $v_n = v_0$. All edges can be represented as $e_i = (v_i, v_{i+1})$, $i = 0, \dots, n - 1$.

Algorithm 1: Integral computation for an arbitrary pair of polygons

Data: Two polygons A and B , a dispersal function ϕ .

Result: Computation of $\text{area}(A \cap (B - t))$ for an arbitrary vector t .

- 1 Compute convex polygons A_1, \dots, A_n such that $A = \bigcup_{i=1}^n A_i$ and such that $\text{area}(A_i \cap A_{i'}) = 0$ if $i \neq i'$;
- 2 Compute convex polygons B_1, \dots, B_m such that $B = \bigcup_{j=1}^m B_j$ and such that $\text{area}(B_j \cap B_{j'}) = 0$ if $j \neq j'$;
- 3 $\mathcal{F} = 0$;
- 4 **for** $i = 1, \dots, n$ **do**
- 5 **for** $j = 1, \dots, m$ **do**
- 6 Increment \mathcal{F} by

$$\int_{\tilde{A}_i \oplus B_j} \text{area}(A_i \cap (B_j - t)) \phi(t) dt;$$

7 **end**

8 **end**

3.1 Area of a convex polygon

A convex polygon can be decomposed into triangles, see Figure 3.1. Thus its area is the sum of its triangles areas. Each of them is computed using the following formula

$$\frac{1}{2}(x_B - x_A)(y_C - y_A) - (x_C - x_A)(y_B - y_A), \quad (3.3)$$

where A , B and C are the triangle vertices and the x 's and y 's are Cartesian coordinates. Equation (3.3) yields a signed area. It is positive if A , B and C are ordered counterclockwise, otherwise it is negative. The final result is exact if the coordinates are integers. The computing time depends on the number of polygon vertices. Algorithm 2 describes the whole procedure. Note that if the polygon vertices are numbered counterclockwise then the triangle vertices are also numbered counterclockwise.

Algorithm 2: Area of a convex polygon. Triangle areas are computed using Equation (3.3).

Data: Convex polygon with vertices (numbered counterclockwise) v_0, \dots, v_{n-1} .

Result: Area of the polygon.

- 1 $a = 0$;
 - 2 **for** $i = 1, \dots, n - 2$ **do**
 - 3 $a = a + \text{area}(\text{triangle } v_0, v_i, v_{i+1})$;
 - 4 **end**
-

For area computation convexity is not an issue. The area of an arbitrary polygon is also easy to compute. If $(x_0, y_0), \dots, (x_{n-1}, y_{n-1})$ are the Cartesian coordinates of the vertices (numbered counterclockwise) of a polygon, its area is equal to

$$\frac{1}{2} \sum_{i=1}^{n-1} (x_i + x_{i+1})(y_{i+1} - y_i). \quad (3.4)$$

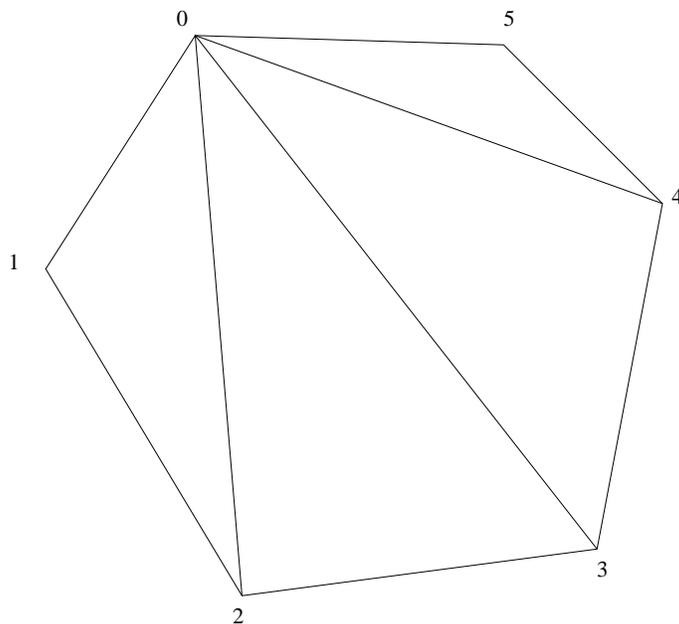


Figure 3.1: Decomposition of a convex polygon into triangles. An arbitrary vertex is connected to all non adjacent vertices.

3.2 Intersection of two convex polygons

Here we focus on the case when the boundaries of the two convex polygons P and Q meet each other: the cases where the intersection is void or where one polygon is included in the other one are not considered.

The intersection $P \cap Q$ is a convex polygon whose vertices are vertices of P or vertices of Q or intersection of edges of P with edges of Q . The intersection can be computed using the algorithm described in [O'R98, Section 7.6]. Two orientated edges $a \subset P$ and $b \subset Q$ are chosen. The edges a and b are advanced so that all the vertices of $P \cap Q$ can be detected and recorded, see Algorithm 3. Note that special cases are not treated: the algorithm is valid if P and Q are in general relative position, i.e. their boundaries cross only at the interior of edges. Also the implementation of this algorithm requires some further low-level functions:

- Test whether two segments meet.
- Compute the intersection of two segments.
- The advancing rule can be reformulated and requires only the computation of signed areas see [O'R98, Section 7.6] for further details.

3.3 Minkowski sum of convex polygons

Let P and Q be two convex polygons. An algorithm for computing the so-called convolution of P and Q is described in [O'R98, Section 8.4]. When both P and Q are convex, the convolution is equivalent to the Minkowski sum. The computation of the convolution is based on the *star diagram*

Algorithm 3: Intersection of two convex polygons

Data: Two convex polygons P and Q
Result: Computation of $P \cap Q$.

- 1 Choose an edge a of P and an edge b of Q ;
- 2 $R = \emptyset$;
- 3 **repeat**
- 4 **if** a meets b **then**
- 5 **if** $a \cap b$ coincides with the first vertex of R **then**
- 6 Terminate;
- 7 **else**
- 8 Add $a \cap b$ to R ;
- 9 **end**
- 10 Advance either a or b ;
- 11 **else**
- 12 **if** One edge points toward the line containing the other **then**
- 13 Advance it;
- 14 **else**
- 15 **if** One edge is on the right-hand side of the other **then**
- 16 Advance it;
- 17 **else**
- 18 Advance either a or b ;
- 19 **end**
- 20 **end**
- 21 **end**
- 22 **until** both a and b cycle along P and Q boundaries;

of P and Q edges. For any edge e of P Let $\alpha(e) \in [0, 2\pi)$ be the angle of e with an arbitrary axis. The star diagram is a polar representation of the α 's. The Algorithm 4 shows how to compute the Minkowski sum from the star diagram. Due to the convexity assumption, α is increasing on the set of edges of a polygon if the reference axis is parallel to its first edge.

Algorithm 4: Minkowski sum of two convex polygons.

Data: Two convex polygons P and Q .
Result: The Minkowski sum $P \oplus Q$.
// Star diagram
1 Compute α for all edges of P and Q taking as the reference axis a line parallel to the first edge of P ;
2 Sort the α 's: $\alpha_k, k = 0, \dots, n + m - 1$ where n is the number of P -vertices and m is the number of Q -vertices;
3 $R = \{\text{first vertex of } P\}$;
4 **for** $k = 0, \dots, n + m - 1$ **do**
5 Add to R the latter vertex of R translated by \vec{e} where e is the edge associated with α_k ;
6 **end**

3.4 Convex partitioning of a polygon

In order to implement Algorithm 1, one needs to decompose an arbitrary polygon into convex polygons. The decomposition algorithm is three-step:

1. The polygon P is triangulated using an ear removal algorithm, see e.g. [O'R98, Section 1.6].
2. Essential diagonals of the triangulation are identified.
3. The convex subpolygons are created.

An internal (resp. external) diagonal is a segment joining two vertices which is contained in (resp. lies outside) the polygon. An ear is a triangle inside the polygon whose vertices are three consecutive vertices a, b, c of the polygon, i.e. ac is an internal diagonal.

The triangulation algorithm, see Algorithm 5, consists in successive ear removals. In order to test whether a vertex v_i is an ear tip, one tests whether $v_{i-1}v_{i+1}$ is an internal diagonal. The latter test is decomposed into two steps: first test whether $v_{i-1}v_{i+1}$ is a diagonal (internal or external), second test if $v_{i-1}v_{i+1}$ is internal. The first test involves edge intersection tests (loop along the edges). For the second test, one has to consider two cases: v_i is convex or reflex. The second test requires only computation of signed areas.

The triangulation yields internal diagonals (inner edges of the triangulation). A non-essential diagonal divides two adjacent cells whose union is still convex. It is easy to check that a diagonal is non-essential if both its ends are convex.

The last step is to split the polygon according to computed essential diagonals, see Algorithm 6.

Algorithm 5: Triangulation of a polygon.

Data: A polygon P with vertices v_0, \dots, v_{n-1} .
Result: A triangulation of P
// Find ear tips
1 **for** $i = 0, \dots, n - 1$ **do**
2 **if** $v_{i-1}v_{i+1}$ is an internal diagonal **then**
3 Set v_i as an ear tip;
4 **end**
5 **end**
6 $T = \emptyset$;
7 $v =$ first vertex of P ;
8 **while** P has more than 3 vertices **do**
9 **if** v is an ear tip **then**
10 Add to T the triangle uvw where u is the vertex previous to v and w is the vertex next to v ;
 // Update ear tip status of u and w
11 **if** the vertices before and after u form a diagonal **then**
12 Set u as an ear tip;
13 **end**
14 **if** the vertices before and after v form a diagonal **then**
15 Set v as an ear tip;
16 **end**
17 Remove v from P ;
18 **end**
19 Advance v ;
20 **end**

Algorithm 6: Creation of convex polygons from the essential diagonals

Data: A nonconvex polygon: its n vertices and $ndiagonals$ diagonals; the essential diagonals are marked. The sides of the polygon are essential diagonals.
Result: The np convex subpolygons: their vertices are stored anticlockwise in $polyg$.
1 $np = 0$
2 **while** there is an essential diagonal **do**
3 $(v_a, v_b) =$ any essential diagonal
4 $start = v_a$
5 **while** $vb! = start$ **do**
6 store (v_a, v_b) into $polyg[np]$
7 mark (v_a, v_b) non-essential
 // Determine the following diagonal:
8 (v_b, v_c) is the diagonal starting from v_b and such as the angle (v_a, v_b, v_c) is minimum
9 $v_a = v_b; v_b = v_c$
10 **end**
11 $np = np + 1$
12 **end**

Chapter 4

Two-dimensional Numerical Integration

This chapter is devoted to the numerical computation of integrals of the type

$$\int_{\check{A} \oplus B} \text{area}(A \cap (B - t)) \phi(t) dt, \quad (4.1)$$

where A and B are bounded polygons and ϕ is an arbitrary integrable dispersal function. As seen in Chapter 3, without loss of generality we can focus on the case when both A and B are convex.

We will start by preliminary remarks concerning the smoothness of the integrand. Then we will discuss two methods for numerical integration:

- A simple randomized discretization of the integral;
- An adaptive cubature method.

The first method, described in Section 4.2, combines simple discretization and Monte-Carlo techniques. This method is quite robust (convergence even for non-smooth integrands). It yields unbiased estimates and it is able to assess its precision. However it may be slow compared to other methods.

The second method consists of an adaptive cubature. First, the domain of integration (a convex polygon) is triangulated. Then the integral over each triangle is approximated using the adaptive cubature method proposed by Berntsen and Espelid [BE92]. The convergence of this method depends on the smoothness of the integrand. It may fail to converge if the integrand cannot be approximated locally by a polynomial. Some basic results about the smoothness of the integrand in Equation (4.1) are stated in Section 4.1. Details about the adaptive cubature method are provided in Section 4.3.

4.1 Smoothness of the integrand

The integrand in Equation (4.1) is the product of two functions:

$$\text{area}(A \cap (B - t)) \text{ and } \phi(t).$$

The function $t \mapsto \text{area}(A \cap (B - t))$ is a piecewise linear function. Its support $\check{A} \oplus B$ can be split by line segments obtained by adding edges of \check{A} and edges of B , see Figure 4.1. Inside each cell of

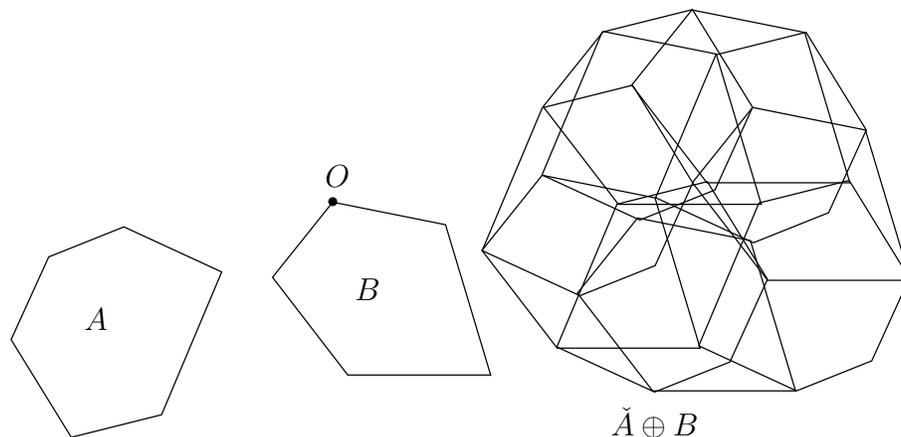


Figure 4.1: Partitioning of the Minkowski sum of two convex polygons A and B according to their edges.

this partition, $t \mapsto \text{area}(A \cap (B - t))$ behaves linearly. The differential $t \mapsto \text{area}(A \cap (B - t))$ is not continuous along the network of cell boundaries.

The smoothness of the whole integrand also depends on the smoothness of the dispersal function ϕ . For instance, the dispersal function given in Equation (15.2) is infinitely continuously differentiable except at the origin where it is not twice differentiable. Then the whole integrand is infinitely continuously differentiable except along the cell boundaries in the partition of the Minkowski sum where it is not differentiable and at the origin where it is not twice differentiable. Another example: the dispersal function given in Equation (15.1) is not differentiable at the origin and it is not twice differentiable along a circle with radius 1.5 meter centered at the origin. Then the whole integrand is not differentiable neither at the origin nor along the cell boundaries and it is not twice differentiable along the circle.

4.2 Method based on grids of points

A simple and intuitive method to perform numerical integration consists of evaluating the integrand over a regular grid of points. The integral is then approximated by summing the integrand over the grid points, and by multiplying the result by the volume of each cell in the grid. Provided the grid position is randomised, this method yields an unbiased estimate of the integral. In addition, it can be repeated several times, with grid positions randomised independently. The integral is then estimated by the mean over the replicated grids. Replications increase precision but also allow the standard error to be estimated.

To simplify, this method will be called **the grid method** in the sequel. In `CaliFloPP`, the distances between the nodes of the grids are the same for all grids and they are chosen by the user. The number of replications is also set by the user.

Let A and B be two polygons. The main steps are :

1. calculation of the Minkowski sum $\check{A} \oplus B$;
2. determination of the smallest rectangle which includes the Minkowski sum and whose sides are parallel to the axes (see Fig. 4.2) ;

3. integration over this rectangle, with the integrand multiplied by a coefficient w equal to 1 if the point is in the Minkowski sum, to 0 otherwise.

Integration is performed as mentioned above, using several grids of points with the following properties :

- all grids have the same x and y lags between adjacent nodes, chosen by the user ;
- each grid is positioned randomly on the integration area, by shifting it randomly relatively to the origin. The shifting is determined by pseudo-random numbers from the uniform distributions over the intervals $[0, p_x]$ and $[0, p_y]$, where p_x and p_y denote the x and y lags between adjacent grid nodes.

The integral is estimated by the mean integral over the replicated grids.

4.2.1 Additional results

- **Standard deviation**

The **standard deviation** is defined as :

$$\text{sd} = \frac{\sqrt{\sum_{i=1}^r (a_i - a_{\bullet})^2}}{r - 1} \quad (4.2)$$

where a_i is the integral value calculated by replication i , and r the number of grid replications.

- **Coefficient de variation**

The **coefficient de variation** is defined as :

$$\text{CV} = \frac{\text{sd}}{a_{\bullet}} \quad (4.3)$$

- **Precision and confidence intervals**

Precision and confidence intervals can be calculated by the user from the replications results. For example, when the number of replications is large enough and the distributions are symmetric, they can be calculated from the quantile of the Student distribution. The half-range hr of the confidence interval, or the absolute precision, is then defined as :

$$\text{hr} = \text{sd} \times \frac{\text{qt}(r - 1, p)}{\sqrt{r}} \quad (4.4)$$

where $\text{qt}(n, p)$ is the quantile for probability p of the Student distribution with n degrees of freedom. The relative precision is $\frac{hr}{a_{\bullet}}$.

4.3 Adaptive cubature method

The cubature method over triangles DCUTRI [BE92] uses an integration rule of degree 27 based on 37 points. Using estimates of approximation errors, triangles are iteratively split into subtriangles until a nominal error is reached. At each iteration the triangle with the largest error is selected for further splitting. The procedure is expected to converge if the integrand is smooth enough inside each triangle. For instance, if the dispersal function is singular at the origin and if the domain of integration $\check{A} \oplus B$ contains the origin, one expects a quicker convergence when the origin is a vertex of the triangulation. Hence (see Figure 4.3):

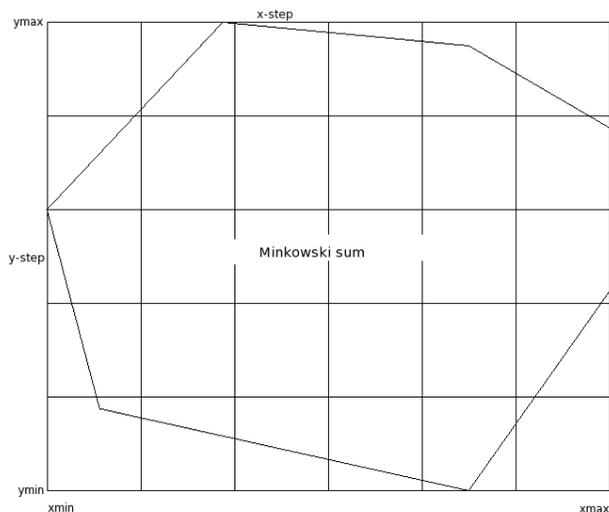


Figure 4.2: Minimal rectangle including the Minkowski sum and grid of points before random shifting

- if $\check{A} \oplus B$ does not contain the origin, it is triangulated from an arbitrary vertex,
- if $\check{A} \oplus B$ contains the origin O , it is triangulated from O .

A further refinement is to avoid to integrate over areas where the dispersal function is considered as negligible that is below a chosen threshold r_{\max} . Note that whenever the dispersal function is non-negative and tends to 0 at infinity, it can be considered in practice as null when it is less than the smallest positive number greater than zero for the used type of number. Thus instead of integrating over the whole Minkowski sum $\check{A} \oplus B$, one may integrate only on its intersection with a disc centered at the origin and with radius r_{\max} . In practice it is simpler to replace the disc by a regular polygon e.g. an octagon containing it, see Figure 4.4. Hence integration is still performed on a convex polygon.

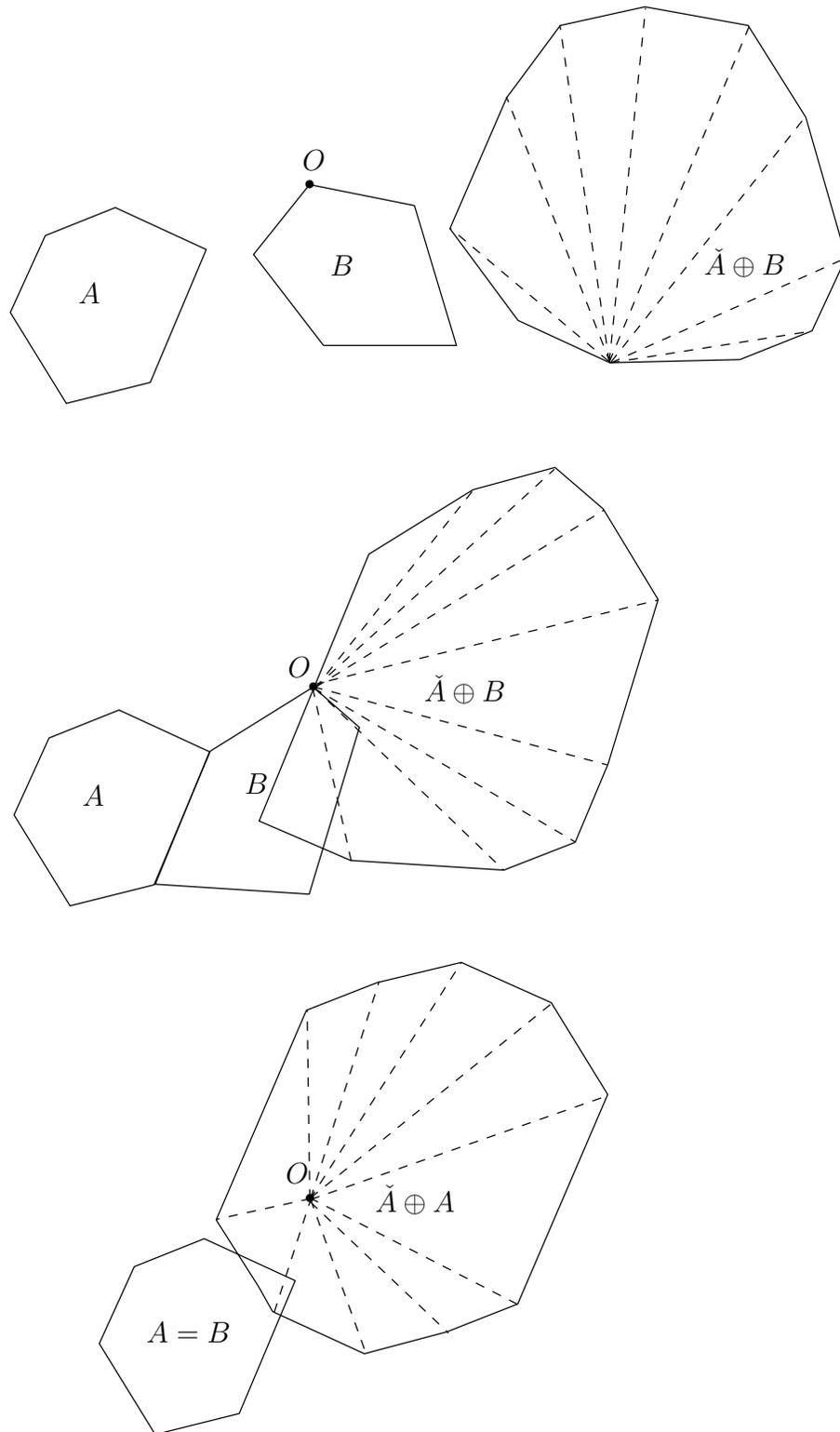


Figure 4.3: Triangulation of the Minkowski sum of two convex polygons A and B . If A and B are disjoint (top), the Minkowski sum $\check{A} \oplus B$ does not contain the origin and is triangulated from an arbitrary vertex. If A and B share a common edge (middle) or if $A = B$ (bottom), the Minkowski sum $\check{A} \oplus B$ contains the origin O and is triangulated from O .

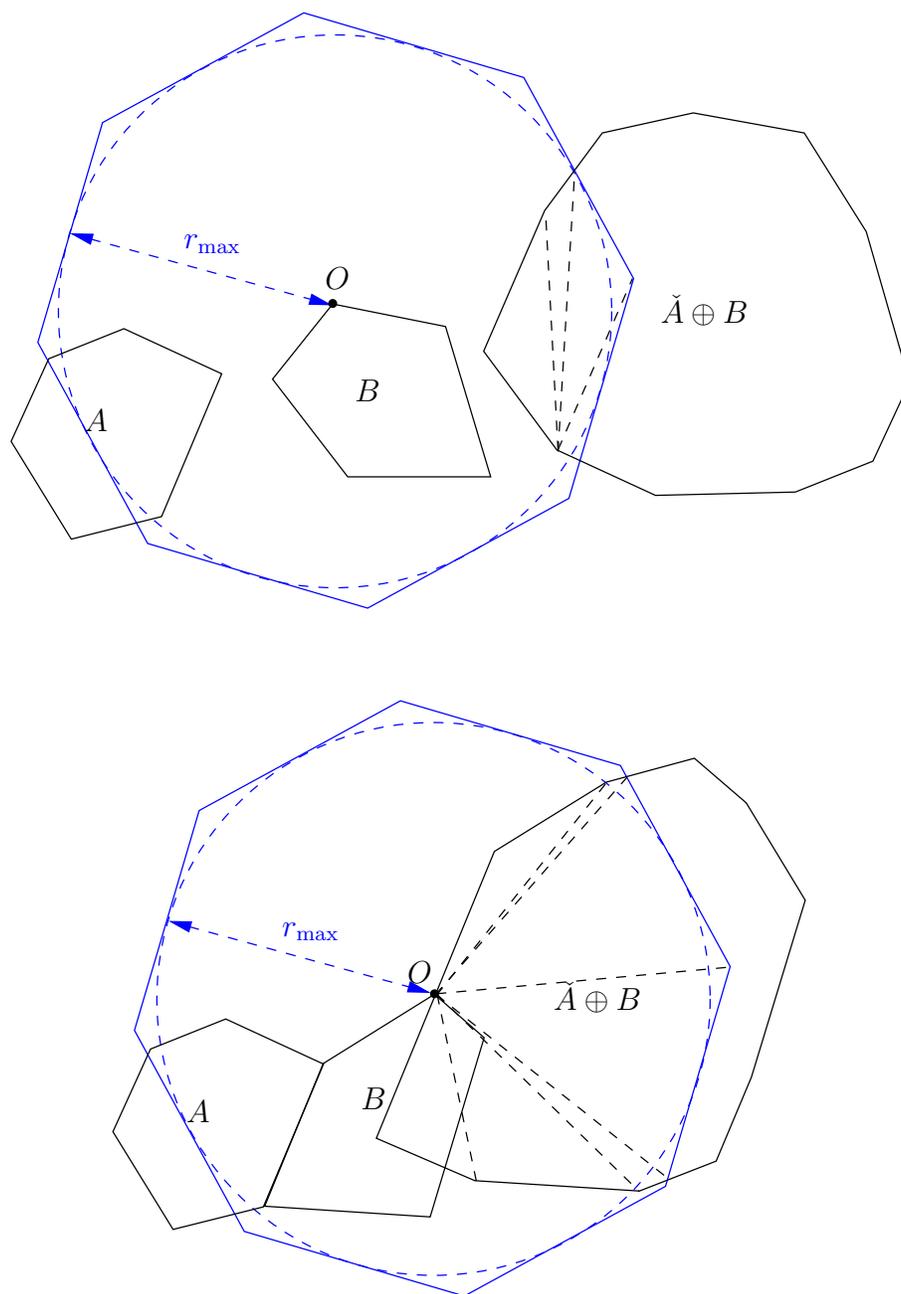


Figure 4.4: Reduction of the domain of integration. Beyond r_{\max} the dispersal function is considered as negligible. The integral is computed only over the intersection of $\hat{A} \oplus B$ and an octagon (blue solid line) containing the disc centered at the origin with radius r_{\max} (blue dash line). Top: the Minkowski sum $\check{A} \oplus B$ does not contain the origin. Bottom: the Minkowski sum contains the origin.

Part II

Example

Chapter 5

Example

5.1 Introduction

In this Section, we analyze the behavior of the grid and cubature methods on a real landscape. First, we compare the results calculated with different parameterisations of each method; then, the two methods are compared.

5.1.1 Data

The data are 66 polygons extracted from the ORTHO demo, a IGN¹ data base , see Fig. 5.1. To illustrate contrasted situations, five pairs of polygons are treated:

- (1,1): two identical convex polygons,
- (14,14): two identical non-convex polygons,
- (11,12): two convex polygons next to each other,
- (56,57): two polygons next to each other, one convex, the other non-convex,
- (4,4): two identical very irregular polygons.

The individual dispersal function is the oilseed rape pollen dispersal function defined in Section 15.2.1.

5.2 Influence of the parameterisation in the grid method

In the grid method, two parameters must be chosen according to the user's needs: the number of replications and the grid step.

5.2.1 Influence of the number of replications

To compare the results calculated with different numbers of replications, four values were successively applied: $r = 5, 10, 15, 20$. The grid step was constant and equal to 1 m for both axes.

¹Institut Géographique National: http://www.ign.fr/rubrique.asp?rbr_id=1619

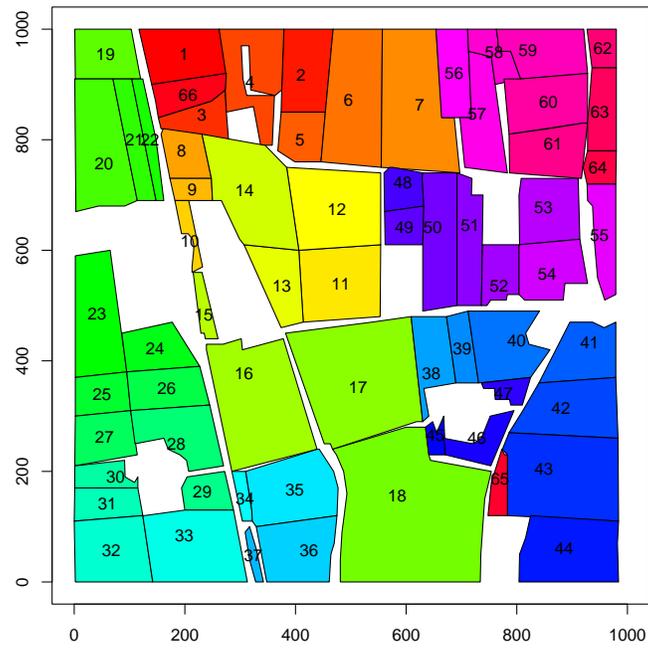


Figure 5.1: Example of 66 polygons extracted from the ORTHO IGN data base. Unit is meter.

Table 5.1: Grid results with different numbers of replications (r) and grid step equal to 1 m.

Polygons	r	$\widehat{\mathcal{F}}$	$\widehat{\sigma}$	$\widehat{\sigma}/\widehat{\mathcal{F}}\times 100$	Times
1↔1	5	12222.2	234.6	1.88	3.5
	10	12282.5	217.7	1.77	7.0
	15	12238.8	204.1	1.66	10.5
	20	12247.7	220.9	1.80	14.1
14↔14	5	23542.1	461.6	1.96	31.9
	10	23359.0	391.1	1.67	63.7
	15	23411	344.4	1.47	95.3
	20	23413.3	332.4	1.41	126.7
11↔12	5	164.5	2.4	1.48	7.0
	10	166.1	3.1	1.89	14.0
	15	167.3	3.1	1.85	21.1
	20	167.2	3.1	1.84	27.9
56↔57	5	132.5	2.0	1.51	5.9
	10	133.0	2.2	1.70	11.7
	15	132.5	2.1	1.62	17.6
	20	132.8	1.9	1.49	23.4
4↔4	5	14610.1	72.3	0.5	45.7
	10	14570.9	91.5	0.62	90.7
	15	14617.7	155.2	1.06	136.7
	20	14631.5	151.5	1.03	181.2

The results² are given in Table 5.1. They are: the evaluated mean flow ($\widehat{\mathcal{F}}$), the standard deviation ($\widehat{\sigma}$), the coefficient of variation ($\widehat{\sigma}/\widehat{\mathcal{F}}$) and the execution time³. We can notice that the execution times are the longer as the polygons are the more irregular: calculation is faster on convex polygons (1↔1, 11↔12) than on non convex ones (14↔14, 56↔57) and very much longer on irregular polygons (4↔4).

5.2.2 Influence of the grid step

To compare the results calculated with different grid steps, four values were tried successively: $step = 0.25$ m, 0.5 m, 0.75 m and 1 m. The number of replications, r , is set to 10.

The results are displayed in Table 5.2. As expected, the times increase as the steps become smaller.

5.3 Influence of the parametrization in the cubature method

In the cubature method, two parameters must be chosen: the maximum number of function evaluations and the precision.

5.3.1 Influence of the number of evaluations

We compare the results calculated with different numbers of evaluations: $Neval = 10^6$, 10^5 , 75×10^3 , 5×10^4 .

²Results are dependent on the random numbers generator; so, actual values may be slightly different.

³ Execution times depend on the material context. They have been observed here on a Dell Biprocessor, in shared mode and 3,2GhZ.

Table 5.2: Grid results with different steps ($r = 10$);

Polygons	step	\mathcal{F}	$\hat{\sigma}$	$\hat{\sigma}/\mathcal{F} \times 100$	Times
1 \leftrightarrow 1	1	12282.5	217.7	1.77	7.0
	0.75	12196.9	27.3	0.22	12.6
	0.5	12277	32.8	0.26	28.5
	0.25	12273.8	4.08	0.03	111.5
14 \leftrightarrow 14	1	23359.0	391.1	1.67	63.7
	0.75	23362.7	183.2	0.78	114.5
	0.5	23376.7	63.4	0.27	258.5
	0.25	23380.6	7.7	0.03	1016.6
11 \leftrightarrow 12	1	166.1	3.1	1.89	14.0
	0.75	167.2	1.4	0.85	25.3
	0.5	167.1	0.5	0.34	57.1
	0.25	167.2	0.1	0.05	223.9
56 \leftrightarrow 57	1	133.0	2.26	1.70	11.7
	0.75	132.5	0.87	0.66	21.1
	0.5	132.5	0.32	0.24	47.8
	0.25	132.5	0.02	0.02	187.5
4 \leftrightarrow 4	1	14570.9	91.5	0.62	90.7
	0.75	14585.4	46.9	0.32	164.5
	0.5	14607.7	14.8	0.10	370.9
	0.25	14612.8	1.85	0.01	1452.8

As the integration process stops as soon as either the maximal number of evaluations or the required absolute or relative precisions are reached, these precisions should be small enough to ensure that all the evaluations are run (here, the required precisions are set to 1.0e-30).

The results are given in Table 5.3⁴ and the confidence intervals are represented in Fig. 5.2. The results obtained by the grid method with a rather great number of replications ($r = 10$) and a small step ($step = 0.25$ m.) are given as references.

5.3.2 Influence of the required precision

To evaluate the impact on the results of the required relative precision, several values were successively tried: $req.rel.er = 0.0001, 0.001, 0.01, 0.1$. The number of evaluations was set to its maximum.

The results are summarized in Table 5.4 and the confidence intervals are represented in Fig. 5.3.

As previously, the results calculated by the grid method with $r = 10$ and $step = 0.25$ m., are given as reference values.

5.4 Global comparison

5.4.1 Global summary

From these computation experiments, some general characteristics can be noticed:

- When the required precision is small enough, the results calculated by the cubature and grid methods are very similar.

⁴ The actual number of evaluations may be slightly less than the required number, because it is a multiple of the number of triangles built by the method on each integration regions.

Table 5.3: Cubature results with different numbers of evaluations. The columns 2 and 3 are grid results ($r = 10, step = 0.25$). The subsequent ones are cubature results with different numbers of evaluations.

Polygons	$\widehat{\mathcal{F}}$	<i>Times</i>	$\widehat{\mathcal{F}}$	<i>rel.er</i>	<i>abs.er</i>	<i>Neval</i>	<i>Times</i>
1↔1	12273.8	111.5	12273.2	2.7e-6	0.033	999962	13.3
			12273.2	3.3e-5	0.4	99974	1.3
			12273.2	4.6e-5	0.57	74962	1.02
			12273.2	5.3e-5	0.65	49950	0.65
14↔14	23380.6	1016.6	23381.1	1.8e-5	0.42	999999	15.1
			23381.4	0.0003	7.7	99863	1.47
			23381.5	0.0006	15.07	74999	1.14
			23379	0.002	54.09	49987	0.72
11↔12	167.2	223.9	167.3	1.3e-6	0.0002	999962	16.8
			167.3	3e-5	0.005	99974	1.6
			166.3	4.2e-5	0.007	74962	1.3
			167.3	8e-5	0.013	49950	0.83
56↔57	132.5	187.5	132.4	5.2e-6	0.0007	999888	17.2
			132.5	0.00010	0.013	99900	1.7
			132.5	0.00016	0.022	74888	1.37
			132.5	0.0005	0.062	49876	0.87
4↔4	14612.8	1452.8	14613.5	5.7e-5	0.8	999888	14.3
			14611	0.0066	96.7	99900	1.4
			14625.6	0.017	249.5	74888	1.15
			14623.9	0.058	849.6	49876	0.73

Table 5.4: Cubature results with different relative precisions required. The columns 2 and 3 are grid results ($r = 10, step = 0.25$). The subsequent ones are cubature results with different relative precisions required.

Polygons	$\widehat{\mathcal{F}}$	<i>Times</i>	$\widehat{\mathcal{F}}$	<i>req.rel.er</i>	<i>rel.er</i>	<i>abs.er</i>	<i>Neval</i>	<i>Times</i>
1↔1	12273.8	111.5	12273.3	0.0001	9.8e-5	1.21	23754	0.3
			12273	0.001	0.00093	11.48	8362	0.1
			12283.4	0.01	0.0098	121.28	5550	0.08
			12279.7	0.1	0.066	820.0	4070	0.06
14↔14	23380.6	1016.6	23381.2	0.0001	9.9e-5	2.3	218707	3.24
			23381.8	0.001	0.00099	23.2	62715	0.9
			23370.4	0.01	0.0099	233.3	30007	0.45
			22762.8	0.1	0.099	2275.2	12395	0.21
11↔12	167.2	223.9	167.3	0.0001	9.9e-5	0.016	42402	0.7
			167.28	0.001	0.00097	0.16	10286	0.2
			166.8	0.01	0.009	1.5	2738	0.05
			166.7	0.1	0.07	12.5	2442	0.05
56↔57	132.5	187.5	132.4	0.0001	9.9e-5	0.013	100344	1.76
			132.3	0.001	0.0009	0.13	16872	0.99
			132.3	0.01	0.0098	1.3	8140	0.19
			132.5	0.1	0.096	12.78	4292	0.08
4↔4	14612.8	1452.8	14613.5	0.0001	9.9e-5	1.46	587708	8.6
			14613.9	0.001	0.0009	14.6	176860	5.16
			14622	0.01	0.0099	145.4	86136	2.17
			14432.3	0.1	0.099	1430.26	38332	1

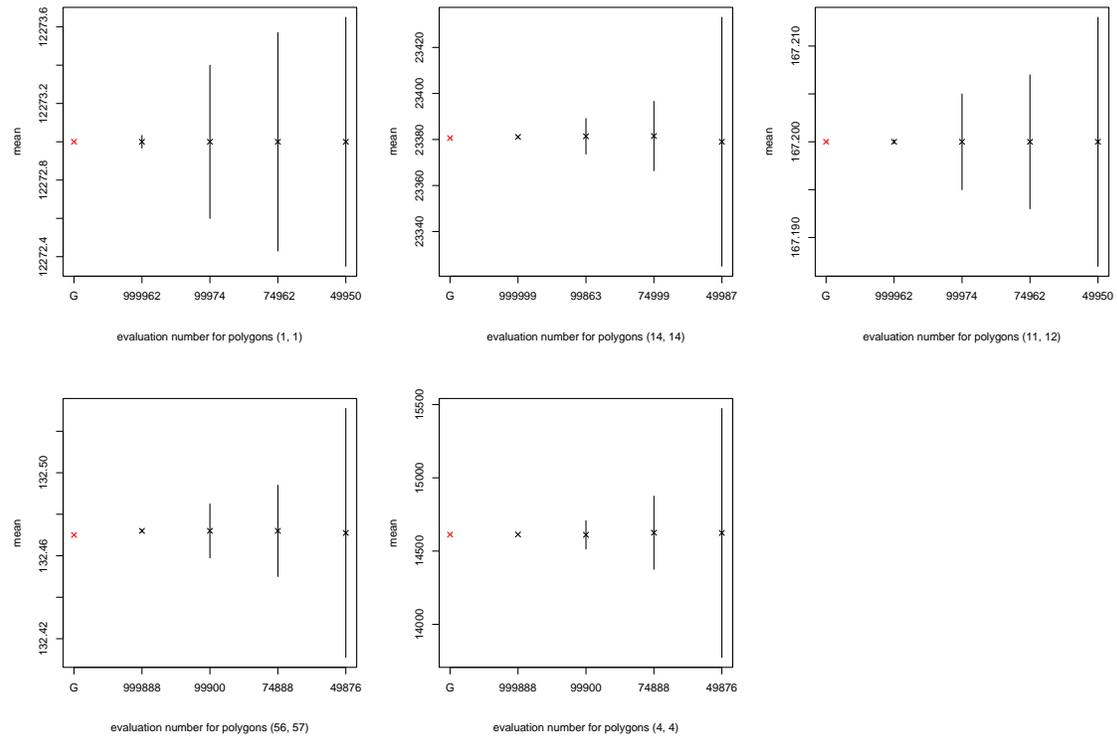


Figure 5.2: Cubature method: Mean and confidence interval against number of evaluations. The first value (abscissa G) is the grid reference value.

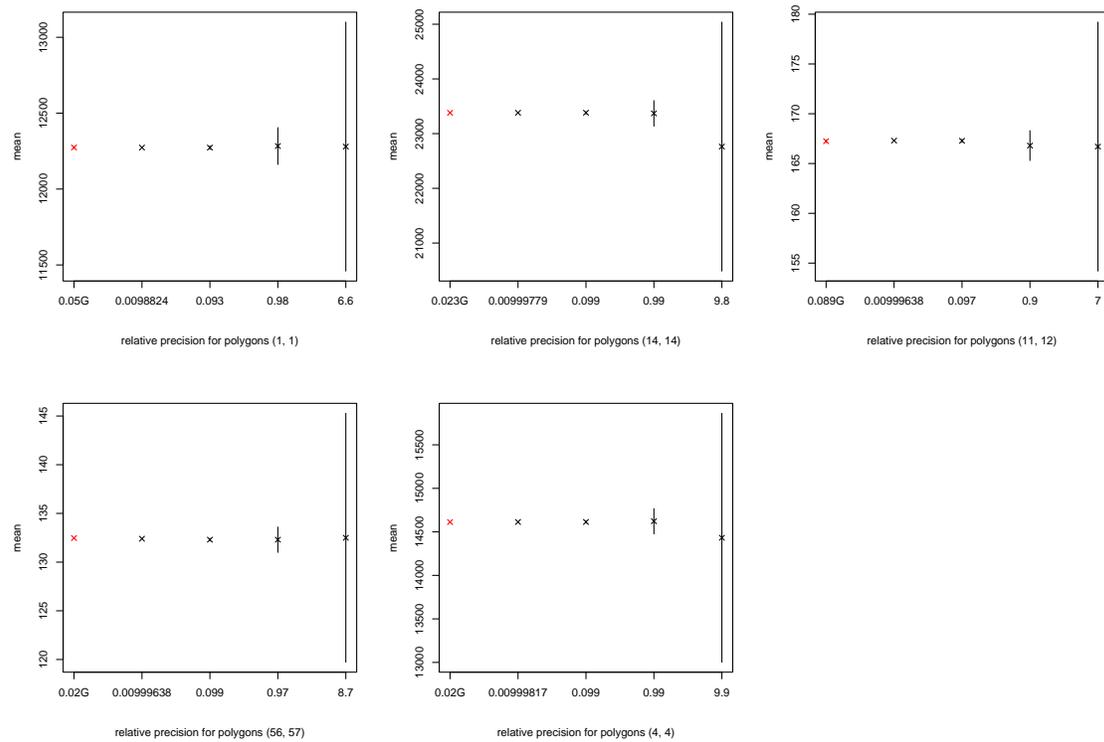


Figure 5.3: Cubature method: Mean and confidence interval against relative precision. The first value (abscissa suffixed by G) is the grid reference value.

- The polygon shape is influent on execution times, in both methods: calculation is faster on convex polygons than on nonconvex ones and very much longer on irregular polygons.
- The cubature method is faster than the grid method.
- In the cubature method, the maximum number of evaluations should be great enough for the precision to be reached. This is all the more so since the polygons are more irregularly shaped. For very irregular polygons, convergence may not be reached, whatever the number of evaluations is.

5.5 Influence of the dispersal function

Section 4.1 has pointed out possible problems when the dispersal function is not smooth (its derivative is not continuous⁵).

To bring into light this behavior, the following non differentiable individual dispersal function is proposed:

$$\phi(t) = \begin{cases} a - b \times t^2 & \text{when } t \leq \sqrt{a/b} \\ 0 & \text{otherwise,} \end{cases}$$

with $a = 10, b = 20$. See Fig. 5.4

All the results calculated by the cubature method on the chosen pairs of polygons are then null except for the pair 4↔4, whatever the required precision is. The grid method gives coherent values.

Comments: Before applying the cubature method on a new dispersal function, it is strongly recommended to compare some results with the ones calculated by the grid method.

5.6 Conclusion

Comparison of the results calculated by the grid and cubature methods on different types of polygons extracted from a real landscape has shown the coherence of these methods. The shapes of the polygons and the required precision of the results have great impact on the execution times with a great advantage for the cubature method. However, the grid method is convenient to provide reference values in case of non convergence or when testing non smooth individual dispersal functions.

⁵ When the dispersal function becomes very suddenly null, the triangles built by the cubature method may intersect the support of the function without any evaluation points being in this support.

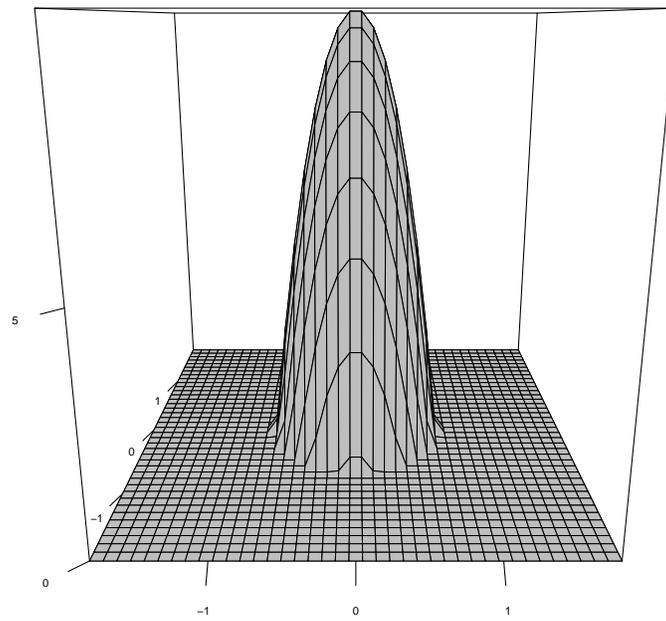


Figure 5.4: Non derivable dispersal function.

Part III

Auxiliary packages

Chapter 6

R Packages

Some R¹ packages may help to prepare the input and visualize output. Two are provided: `Rcaliflopp` and `landm`.

6.1 Rcaliflopp

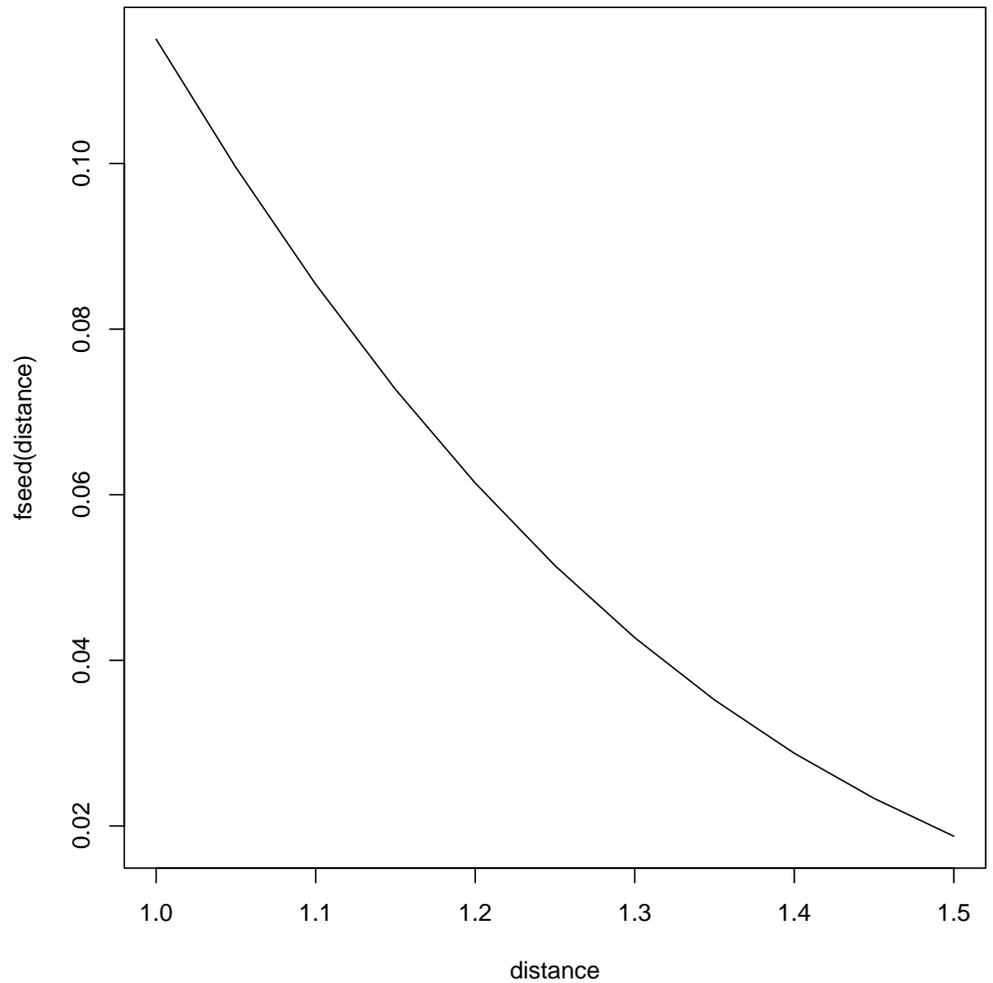
This package provides classes and methods for viewing input and output of the programme `CaliFloPP`.

6.1.1 Example

From a vector of distances, the function `fseed` calculates the individual seed dispersion function used in `CaliFloPP`.

```
distance = seq(1,1.5, by=0.05)
par(pty="s")
plot(x=distance, y = fseed(distance), type="l")
```

¹<http://cran.r-project.org/>



6.2 landm

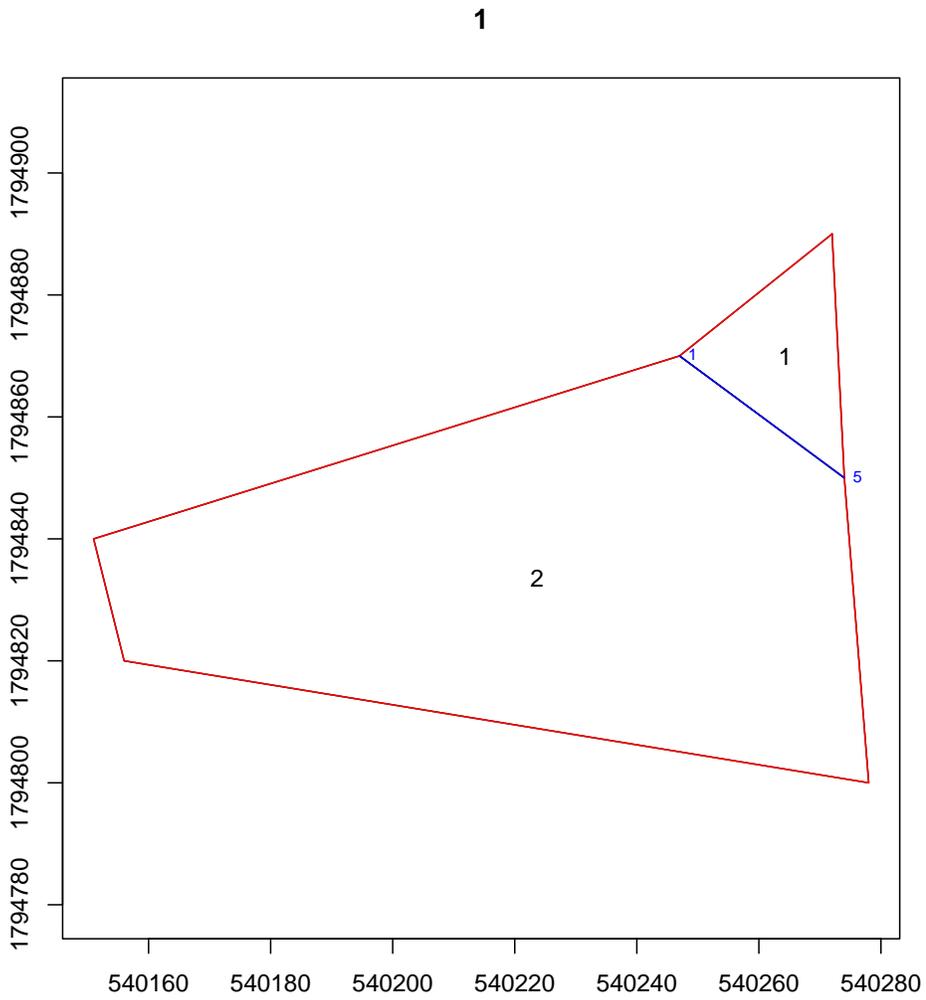
This package enhances the package “sp” for manipulation of objects Polygons-class and Polygon-class (2D polygons): plot, extraction, creation of convex polygons, computation of distances, etc ... See details in the online help-files.

6.2.1 Example

The function `crConvex` splits a non convex polygon into convex subpolygons.

```
p1=Polygon(cbind(c(540272, 540274, 540278, 540156, 540151,  
                  540247, 540272),  
              c(1794890, 1794850, 1794800, 1794820, 1794840, 1794870, 1794890)))
```

```
par(pty="s")  
crConvex(p1, plot=TRUE)
```



Part IV

Installation Guide

Chapter 7

Prerequisite

Licence Agreement: This software is submitted to a Licence Agreement: read the files `COPYING.en` (english version) or `COPYING.fr` (french version) included in the distribution.

Prerequisite: A C/C++ compiler.

Optionally, for installation of additional R-packages, the R system ([\[CRA\]](#)). The package `Rcaliflopp` needs the package `splancs` and the package `landm` needs the package `sp`.

Tested installations: Installation has been tested on Linux Mandrake and Mandriva distributions with the GNU-compiler `g++` and on Windows XP with Dev-C++.

Chapter 8

Installation Steps

1. Unload the tar-archive, uncompress it by the command **gzip** and untar it by the command **tar xf** : a directory named **califlopp-<version>** is then created.

The tar-archive file is about 9Mb compressed and 3Mb uncompressed.

2. Customize the context dependent constants:

See Section 9.

3. Installation:

Two procedures are available

- Installation by the ‘configure’ shell script.

This script attempts to guess correct values for various system-dependent variables used during compilation. In the directory “califlopp”, type:

`./configure` (configure the package for your system)

`make` (compile the package)

`make check` (run tests)

`make install` (install the programs)

`make clean` (remove binaries and object files)

For more details, see the file `INSTALL` or type `./configure --help`.

- Installation by your own configuration.

- (a) Customize the compilation options.

- Performance measurement (CPU or actual elapsed time).

The functions “getrusage” or “times” should be available. In the file `obj/subdir.mk`, comment the appropriate `COPTIONS1` sentence, and uncomment the others.

The function “times” is the default.

- Random number generation.

The functions “drand48” or “rand” or “genrand_real2” should be available. In the file `obj/subdir.mk`, comment the appropriate `COPTIONS2` sentence, and uncomment the others. The function “genrand_real2” is the default.

- (b) Compile:

A makefile is available in the directory `obj`. Place yourself in this directory and type: `make all`.

Notes:

- Type `make clean` before a re-compilation.
 - To compile one programme or one component only, specify the target.
For example: `make surface`.
 - Files suffixed by ".d" contain the dependences between files. For example, the file `surface.d` contains the names of the files needed by `surface.cpp`. These files are automatically created by the `make` command.
- (c) Clean up:
- You can now delete the `obj` directory, but be careful: it contains the `makefile` and `subdir.mk` files required for a re-compilation.
- You can also delete the `src` directory, but be careful: the user may need to know what the dispersal functions are — they are defined in the file `src/functions.cpp` —, and what the valid bounds and default values of the parameters are — they are defined in include files of `src`: see Section 9.
4. Try some examples: see the file `examples/ReadMe.html` and the files `execution` in the `examples` sub-directories.
For example: `cd examples/ex-data; ../../califlopp -i data -p ex.param`.
 5. Optionally, install the R-packages `Rcaliflopp` and `landm`, by using the `INSTALL` command of R. For example, to install `Rcaliflopp`, connect yourself as root and type in:

```
mkdir RCALI
R CMD INSTALL Rcaliflopp_0.0-1.tar.gz
```

(verify the version suffix of the provided `Rcaliflopp.tar` file: 0.0-1 is an example)

Careful: the package `splancs` should have been installed before.

To install the package in your own location, rather than in the standard R library location for which you need special rights, add the option `-l RCALI` into the above command, where `RCALI` is for the pathname of the installation directory. This directory should have been created before.

Do the same, for the R-package `landm`. `landm` requires the package `sp` been installed before.

Chapter 9

Configuration

The file `src/caliconfig.h` contains configuration variables that you should customize according to your needs. The following tables describe these configuration variables.

In the first column, in addition to the variable names, information is given about the possibility for the user to modify the default value: an asterisk means that it is the case in interactive mode, and a word between parenthesis that it is the case in non-interactive mode. This word is then the associated keyword in the parameter-file (see Section [12.2](#)).

9.1 Input

Name	Meaning	Comments
DEFAULT_INPUT_FORMAT (input) (*)	Format of the polygons-file	- should be 1 if each polygon is coded on two lines: 1/ an identification number, followed by the x-coordinates 2/ the same number, followed by the y-coordinates, - should be 2 if each polygon is coded on three lines: 1/ an identification number, a name, the number of vertices (followed possibly by other data that are ignored) 2/ the x-coordinates 3/ the y-coordinates.
DEFAULT_DELIM (delim) (*)	Separator character in the polygons-file	should be between double-quotes
COMMENT	Character introducing comments in the parameter file	
MAX_LINE_POLY	Maximal number of characters on each line of the polygon file	
MAX_NAME	Maximal length of the polygon names	
PATH_MAX	Maximal number of characters for pathnames	usually, PATH_MAX is defined in stdio.h

9.2 Output

Name	Meaning	Comments
OUTPUT_FILE_FORMAT	Content of the result-file	<ul style="list-style-type: none"> - should be ALL to output all the results - should be FLOW to output the polygon identifiers and the flow by square meter, - should be LIGHT to output all the results except for the time.
OUTPUT_WARNING	Warnings output on the error unit	<ul style="list-style-type: none"> - should be ALL to print all warnings, - should be NOTHING for minimum warnings.
DEFAULT_OUTPUT (output)	Output on the standard output unit	<ul style="list-style-type: none"> - should be ALL to print all the results, - should be FLOW to print the integrated flows, the flows by m², - should be LIGHT to print the integrated flows, only, (one line per pair of polygons) - should be NOTHING for no print.
DEFAULT_VERBOSE (verbose) (*)	verbose mode	should be 1 to get output about the decomposition into convex polygons and landscape relocation, and 0 otherwise

9.3 Error treatment

Name	Meaning	Comments
ERR_POLY	treatment of erroneous polygons	<ul style="list-style-type: none"> - should be 0 if an error on a polygon should be a warning: the erroneous polygon is then ignored - should be 1 if an error on a polygon should be fatal

9.4 Landscape features

Name	Meaning	Comments
MAX_VERTICES	Maximal number of vertices per polygon	
MAX_TRIANGLES	Maximal number of convex sub-polygons per polygon	This number depends on the polygons shapes: more they have obtuse angles, more the number of convex subpolygons should be great. But, be careful: If values of MAX_VERTICES and MAX_TRIANGLES are too big, execution errors may occur ("Segmentation fault" or "Out of memory")
TRANSLATE	Landscape relocation.	Should be 1 if the landscape should be systematically relocated, so that the left-bottom corner of the landscape is (1,1). (Recommended value)
SCALE	The polygon-coordinates are multiplied by SCALE.	Should be 1 or a multiple of 10. For example, to take into account centimeters, set SCALE to 100
SAFE	Maximal range of the coordinates	It is the maximal range of the coordinates after they have been multiplied by SCALE. SAFE should be less than INT_MAX (which is usually= 2147483647)
DISTP	When the distance between two successive vertices is less than or equal to DISTP, the second vertex is suppressed.	Expressed in meters.
ANGLEPREC	Precision of the angle between 3 successive vertices.	When the arccosinus of the angle between three successive vertices is inside $[\pi - \text{ANGLEPREC}, \pi + \text{ANGLEPREC}]$, the vertices are considered as aligned, and the second one is suppressed. When it is inside $[-\text{ANGLEPREC}, +\text{ANGLEPREC}]$, it is supposed that the sharp spike they form is an artefact, and the second one is suppressed.

9.5 Individual dispersal functions

Name	Meaning
DEFAULT_NFUNCTIONS (nfunc) (*)	Default number of dispersal functions taken into account. Should be less than or equal to 5. These functions are coded in the file <code>functions.cpp</code> in subroutines named f1, f2,..., f5. (The delivered subroutines are f1 and f2, the pollen and seed dispersal functions of oilseed rape described in this manual).
DZ1, DZ2, DZ3, DZ4, DZ5	Thresholds for dispersal distances: When the minimal distance between two polygons is greater than or equal to these values, the corresponding dispersal function (f1 for DZ1, ... f5 for DZ5) is supposed to be null; distances are in meter. Negative or null values mean that there is no limit in the dispersal.
DP1, DP2, DP3, DP4, DP5	Thresholds for dispersal distances: When the minimal distance between two polygons is greater than or equal to these values, the dispersal is calculated between polygons centroids; distances are in meter.
TZ1, TZ2, TZ3, TZ4, TZ5	Method of triangulation for the cubature method. Should be True, if triangulation from (0,0) has to be done when (0,0) is included in the integration area (recommended value when the dispersal function is very "sharp" at the origin).

9.6 Methods features

Name	Meaning	Comments
DEFAULT_METHOD (method) (*)	Integration method	- should be 1 to set the grid method as the default method, - should be 0 to set the cubature method as the default method.

9.6.1 Grid method

Name	Meaning
MAX_EST	Maximal number of estimations
DEFAULT_EST (r) (*)	Default number of estimations (\leq MAX_EST)
DEFAULT_STEPX (stepx) (*)	Default step on the x-axis grid of points; in meters.
DEFAULT_STEPY (stepy) (*)	Default step on the y-axis grid of points; in meters.
DEFAULT_SEED (seed) (*)	Default value of the seed for the random number generator.

9.6.2 Cubature method

Name	Meaning
DEFAULT_ABS_ERR (abser) (*)	Default absolute precision
DEFAULT_REL_ERR (reler) (*)	Default relative precision
DEFAULT_MAX_PTS	Maximal number of evaluation points per integration region.
DEFAULT_NB_PTS (maxpts) (*)	Default maximal number of evaluations per triangle (should be in [37,DEFAULT_MAX_PTS])
MAX_SREGIONS	Maximal number of subregions per integration region.

9.7 Numerical parameters

Name	Meaning	Comments
REAL_PREC	Precision for real comparisons in geometrical computations	Recommended: (REAL_MIN*1.0e+4)

Chapter 10

More options

Some particular versions can be installed by configuring the file `obj/subdir.mk`, before compiling:

- Precision of the floating point numbers.

By default, the type of the real numbers is `double`. To switch to simple precision (i.e `float`), add to the values of `COPTIONS` : `-DFLOAT`

- Installation of a reduced version.

The reduced version is less memory consuming but can only process the cubature method, in non-interactive mode, and does not allow selection of polygons. If wanted, un-comment in the file `obj/subdir.mk` the sentence: `REDUCED = -DREDUCED`

Part V
User Guide

Chapter 11

Quick Start

1. Non-interactive mode

- Usage:

```
califlopp -i polygons-filename [-p parameter-filename] [-r result-filename]
```

(califlopp.exe instead of califlopp on windows systems).

The square brackets delimit what can be omitted.

- Input arguments:

- polygons-filename: name of an ASCII file which contains the polygons coordinates. The coordinates should be ordered clockwise. The polygons can be closed or not.

The syntax of this file is:

- * on the first line: the number of polygons,

- * on the following lines:

- if `input`¹ = 1, two lines per polygon:

- an identifier - a positive integer - followed by the x-coordinates,

- the same identifier followed by the y-coordinates.

(Careful: no blank character after the last coordinate)

- if `input` = 2, three lines per polygon:

- an identifier - a positive integer - followed by the name of the polygon and by the number of its vertices,

- the x-coordinates,

- the y-coordinates.

See Section 12.1 for more details.

- parameter-filename: name of a file which contains the user's choices. Each line of this file should contain `<keyword><value>` pairs. See Array Section 12.2 as to the valid keywords and their meanings.

When this argument is missing, all the pairs of polygons are treated with the default values of the parameters.

- Output argument:

¹ input is a parameter set in the parameter-file. By default, it is the value of the constant `DEFAULT_INPUT_FORMAT` set in the file `src/caliconfig.h`.

- `result-filename`: name of a file which will contain all or part of the results output for further analysis. See Section 13.2 for details.

2. Interactive mode

In interactive mode, questions are asked to the user. The polygons-file should have been prepared as in non-interactive mode before launching the execution.

- **Usage:**
`califlopp` or `califlopp.exe`
See Section 12.3 for details about the dialogue.

Note: Screen output depend on the parameter `output`² (see Section 13.1): all, part or none of the results are displayed.

²output is a parameter set in the parameter-file. By default, it is the value of the constant `DEFAULT_OUTPUT` set in the file `src/caliconfig.h`.

Chapter 12

Input

12.1 The polygons-file

In accordance with the gene flow application and the dispersal functions defined in Section 15.2, we assume in the following that 1 unit in the polygon coordinates corresponds to 1 m.

12.1.1 Constraints on the polygons

- Polygons should be without holes.
- Small and narrow polygons (approximately less than 1 m²) should be avoided because of possible numerical problems, as well as polygons with many obtuse angles because their decomposition into convex subpolygons may not be possible.
- Shape and size restrictions are set in the file `src/caliconfig.h`. They are:

MAX_VERTICES, the maximal number of vertices per polygon,
MAX_TRIANGLES, the maximal number of convex subpolygons per polygon,
SAFE, the maximal extent of the landscape.

Notes: There is no limit in the number of polygons (except possible memory limitation) and the polygons may intersect.

12.1.2 Syntax of the polygons file

The polygons file contains the coordinates of the polygons. It should respect the following rules:

- It should be an ASCII-file.
- Vertices should be ordered clockwise.
- The polygons may be closed or not.
- The coordinates may be negative or null. The number of decimal digits taken into account depends on the constant `SCALE`¹. (See Section 15.1.1).

¹Constant set in the file `src/caliconfig.h`

- The values separator is the character `DEFAULT_DELIM`¹. In interactive mode, this character cannot be changed. In non-interactive mode, it can be changed by the keyword `delim` in the parameter-file (See Section 12.2).

The separator character can be repeated any number of times between successive values.

- Two formats for the polygons file are catered for: see Section 11.

The default format is defined by the constant `DEFAULT_INPUT_FORMAT`¹. In interactive mode, this format cannot be changed. In non-interactive mode, it can be changed by the keyword `input` in the parameter-file.

- In format 2, the polygon names can consist of several words, as long as these words are not separated by the values separator character.

Note:

If the number of polygons set on the first line, `npoly`, is less than the effective number, only the first `npoly` polygons will be treated.

12.2 Parameter file in non-interactive mode

In non-interactive mode, the user's choices are passed to the programme via a parameter file, the syntax of which is:

- Each main line contains a `<keyword><value>` pair; the keyword and the value can be separated by one or several blank or tabulate characters.
- A default value is associated with each keyword: it is equal to the constant named `DEFAULT_<KEYWORD>` set in the file `src/caliconfig.h`.
- The main lines may be in any order.
- Comments are introduced by the character `#`: this character and the rest of the line are ignored.

Note: The parameter file can be reduced to the only values to be changed; it can even be omitted.

Example of a very simple parameter-file:

```
verbose 1 # verbose output
method 1 # grid method
output 2 # reduced output
```

Keywords and their meanings in the parameter-file:

keyword	value
verbose	1 if output is required about polygons convexity and landscape translation, else 0.
input	format of the polygons file: 1 or 2
delim	separator between values in the polygons-file: given as a character between double-quotes.
output	output required on the screen: 0 nothing, 1: all results, 2: progression numbers, 3: the integrated flows and their means per m ² .
nfunc	number of required dispersal functions. On the following line, type nfunc integers: 1 is for the dispersal function implemented in the subroutine “f1” in the file <code>/src/functions.cpp</code> , 2 is for the “f2” subroutine, and so on.
method	integration method: 1: grid, 0: cubature
seed (grid method)	seed of the random generator
stepx (grid method)	step of the grid on the x-axis in meter
stepy (grid method)	step of the grid on the y-axis in meter
nr (grid method)	maximal number of replications or grids
maxpts (cubature method)	this keyword should be followed by the index of a dispersal function. On the following line, type the maximal number of evaluation points required for this function. (See also maxpts Section 12.3.)
reler (cubature method)	this keyword should be followed by the index of a dispersal function. On the following line, type the maximal relative error required for this function.
abser (cubature method)	this keyword should be followed by the index of a dispersal function. On the following line, type the maximal absolute error required for this function.

To specify the required polygons in the parameter-file:

When only one pair of polygons should be treated, indicate the numbers of these polygons on two lines:

keyword	value
poly1	identifier of the first polygon.
poly2	identifier of the second polygon.

When several pairs should be treated, there are two possibilities:

keyword	value
1. ncouples	number of required pairs of polygons. This line should be followed by ncouples lines, each of them with the two identifiers of the polygons of one pair.

	keyword	value
2.	nwant	number of source or target polygons. This line should be followed by a line with the <code>nwant</code> polygons identifiers: their flows to (or from) all the others will be calculated.

Example of parameter-file

```

verbose 0 # no verbose output
input 1   # format 1 of the polygons-file
delim " " # values separator on the polygons-file
output 2  # reduced screen output
method 0  # the cubature method
maxpts 1  # for function 1 (pollen dispersal),
300000   # set the maximal number of evaluation points
maxpts 2  # for function 2 (seed dispersal),
10000    # set the maximal number of evaluation points
abser 2   # for function 2 (seed dispersal),
0.01     # set the required absolute precision
ncouples 2 # only two pairs of polygons
1 1      # the first pair
25 30    # the second pair

```

12.3 Dialogue in interactive mode

When invoked without argument, the command `califlopp` (or `califlopp.exe`) opens a dialogue with the user. Some explanations may help to answer the questions:

- **verbose reading:** if `y` (yes), information is given about the decomposition of the non-convex polygons into convex ones, and about the translation of the landscape.
- **Do you want to store the results on file? (y/n)**
 - **pathname prefix of the output file:**
 If `y` (yes) and `myfile` are the answers to these questions, two files are created or replaced: the file `myfile.grid` contains the results by the grid method, and the file `myfile.cub` the results by the cubature method. Structures and contents of these files are described in Section 13.2.
- **Questions about the grid method:**
 - **Number of estimations?** The number of estimations is the number of grid generations, or replications.
 - **Seed of the random generator:** By setting the same value for different runs with identical input, identical results are obtained.
- **Questions about the cubature method:**
 - **Precisions (absolute and relative):** The user can set thresholds for the precisions, and so, stop the integration process as soon as one of them is reached. In any case, the integration process stops when the maximal number of evaluations is reached.
 - **maximal number of evaluations:** Integration process stops when this number of evaluations is reached, whatever the results precision is.

If the value answered by the user is too small or too large, it is automatically corrected. Let $reqmaxpts$ be this value and $ntri$ be the number of triangles the current region is composed of, the effective maximal number of evaluations, $maxpts$, is:

- * $maxpts = reqmaxpts$, if $37 \times ntri \leq reqmaxpts \leq \text{DEFAULT_MAX_PTS}$ ²
- * $maxpts = 37 \times ntri$, if $0 < reqmaxpts \leq 37 * ntri$
- * $maxpts = \text{DEFAULT_NB_PTS}$ ² $\times ntri$, if $reqmaxpts \leq 0$,
- * $maxpts = \text{DEFAULT_MAX_PTS}$, if $reqmaxpts > \text{DEFAULT_MAX_PTS}$.

²Constant set in the file `src/caliconfig.h`

Chapter 13

Output

13.1 Screen output

Screen output depend on the parameter `output` set in the parameter-file or, by default, on the constant `DEFAULT_OUTPUT`¹. For each pair of polygons:

- When `output=1` or `DEFAULT_OUTPUT=ALL`, output are:
 - With the grid method:
 - * the integrated flow calculated at each replication,
 - * the final value of the **integrated flow**, its mean per m² of both polygons, the **standard deviation** and the **variation coefficient**.
 - With the cubature method:
 - * the **integrated flow**, its mean per m² of both polygons, the absolute error, the **confidence interval** and the number of evaluations.
An asterisk before the absolute error means that the convergence has not been reached with the required precision.
 - With both methods, the areas of the polygons.
- When `output=2` or `DEFAULT_OUTPUT=LIGHT`, an iteration number (starting from 1) is only the output.
- When `output=3` or `DEFAULT_OUTPUT=FLOW`, output consist of: the integrated flow and its mean per m² of both polygons.
- When `output=0` or `DEFAULT_OUTPUT=NOTHING`: nothing is written.

Note: When all the pairs of polygons are treated, only $(npoly*(npoly+1))/2$ results are displayed, where *npoly* is the number of polygons. Indeed, dispersals are symmetric.

Examples of output can be found in files suffixed by `.out`, in the subdirectories of the `examples` directory.

¹Constant set in the file `src/caliconfig.h`

13.2 Result file

On the result-file:

- The values are separated by tabulates.
- The first line contains:
 - "npoly" followed by the number of polygons, "input-file" followed by the name of the polygons file, "nfunc" followed by the number of dispersal functions, and at last, "method" followed by the name of the integration method, i.e. "cubature" or "grid".
- The content of the following lines depends on the constant OUTPUT_FILE_FORMAT²:
 - when OUTPUT_FILE_FORMAT= ALL, all the results are written on the file;
 - when OUTPUT_FILE_FORMAT= LIGHT, the execution times are not written;
 - when OUTPUT_FILE_FORMAT=FLOW, the flows per m² are written only.

More precisely, there are one or several lines, \mathcal{L} , for each pair of polygons:

- The first line contains:
 - * the identifiers of both polygons;
 - * for each dispersal function, the integrated flow divided by the area of the second polygon;
 - * when OUTPUT_FILE_FORMAT =ALL or =LIGHT, the areas of both polygons;
 - * when OUTPUT_FILE_FORMAT =ALL or =LIGHT, eventually, results specific to the cubature method, (see below);
 - * when OUTPUT_FILE_FORMAT =ALL, the execution time in milli-seconds.
- When the first polygon and the second one are different (i.e when the flow is not from a polygon to itself), the following line contains the same information, with the first and second polygons inverted.
- When OUTPUT_FILE_FORMAT =ALL or =LIGHT and the method is grid, this line is followed by one line with the x-axis and y-axis grid steps and the number of evaluations, then by as many lines as dispersal functions, each one with:
 1. the **integrated flow**,
 2. the **standard deviation**,
 3. the number of replications, **nr**,
 4. "**r:**" followed by the **nr** results.
- When OUTPUT_FILE_FORMAT =ALL or =LIGHT and the method is cubature, the results specific to the cubature method are written on the first line of \mathcal{L} . For each dispersal function, output are:
 1. the **integrated flow**,
 2. the bounds of the **confidence interval**,
 3. the **absolute error**,
 4. the number of evaluations.

Examples can be found in files suffixed by `.res`, in the subdirectories of the `examples` directory.

² Constant set in the file `src/caliconfig.h`. The user has no possibility to modify the value of OUTPUT_FILE_FORMAT.

13.3 Error treatment

When an error is encountered, an explicit message is issued on the standard error unit (the screen, by default). Some types of errors are treated specifically:

- **Error in a polygon:**

A polygon is considered as not valid when it cannot be split into convex subpolygons, i.e. when it has too many obtuse angles.

- In the auxiliary programmes (see Section 16), an error message is issued, and the polygon is ignored.
- Elsewhere, the treatment depends on the constant `ERR_POLY`³. When `ERR_POLY` is null, an error message is issued, and the polygon is ignored. Otherwise, the error is fatal.

- **Memory allocation problem, Overflow and Range Error:** An error message is issued and execution stops and returns a negative value.

³Constant set in the file `src/caliconfig.h`

Chapter 14

Example

The names of the executables are supposed here suffixed by “.exe” (windows version).

14.1 Polygons file

The polygons file is named `data`. It is in format 1 and the separator character is the blank character. Its first lines are:

```
66
1 540139 540116 540261 540274
1 1794900 1795000 1795000 1794920
2 540378 540467 540453 540373 540374
2 1795000 1795000 1794850 1794850 1794890
```

14.2 Calculation by the cubature method

14.2.1 Parameter file

Only one result is calculated here: the integrated flow from the polygon 66 to itself, by the cubature method. Thresholds are required for the relative errors: 1.0e-4 for function 1 (pollen flow) and 1.0e-3 for function 2 (seed flow). The other parameters are let to their default values. The parameter file, named `ex.param`, is:

```
output 1      # maximal output
input 1       # polygons-file in format 1
delim " "    # separator character on the polygons-file
reler 1       # for function 1 (pollen dispersal),
1.0e-4       # require a relative precision
reler 2       # for function 2 (seed dispersal),
1.0e-3       # require a relative precision
poly1 66     # integrated flow from polygon 66 to itself
poly2 66
```

14.2.2 Command line

The command line is:

```
califlopp.exe -i data -p ex.param -r ex.res
```

14.2.3 Screen output

On the screen, maximal output are displayed:

```
Parameters:
-----
verbose: 0
output: 1
scale: 1
method:cubature
function 1: relative precision = 0.0001, absolute precision = 0.001
function 2: relative precision = 0.001, absolute precision = 0.001
poly1: 66
poly2: 66
```

```
Polygons n° 66, 66
-----
```

Elapsed time in integration: 880 milliseconds.

```
Integrated flow for function 1:
mean: 6117.53 mean/area1: 0.942609 mean/area2: 0.942609
absolute error: 0.6102 confidence interval: [6116.92, 6118.14]
nb. evaluations: 69412
```

```
Integrated flow for function 2:
mean: 6403.69 mean/area1: 0.9867 mean/area2: 0.9867
absolute error: 5.80628 relative error: 0.000906709
confidence interval: [6397.88, 6409.49]
nb. evaluations: 14430
```

```
area1: 6490 area2: 6490
```

14.2.4 Output on the result-file

The file `ex.res`¹ contains two lines. The first one identifies the input. The second one contains the identifiers of the polygons and the pollen and seed integrated flows per m².

```
npoly: 66 input-file: data nfunc: 2 method: cubature
66      66      0.942609      0.986552
```

14.3 Calculation by the grid method

14.3.1 Parameter file

The parameter-file, `exg2.param`, is:

¹OUTPUT_FILE_FORMAT is here equal to FLOW; see Section 13.2.

```

output 1      # maximal output
input 1      # polygons-file in format 1
delim " "    # separator character on the polygons-file
poly1 66     # integrated flow from poly 66 to itself
poly2 66
method 1     # method grid
stepx 0.25   # grid steps
stepy 0.25
nr 20        # number of repetitions

```

14.3.2 Command line

The command line is:

```
califlopp.exe -i data -p exg2.param -r exg2.res
```

14.3.3 Screen output

Final results on the screen are:

```

Elapsed time in integration: 312280 milliseconds
Nb. evaluations: 43628800

```

```

Integrated flow for function 1:
mean: 6117.35 mean/area1: 0.942581 mean/area2: 0.942581
standard deviation: 1.29958
coefficient of variation (std/mean): 0.000212442

```

```

Integrated flow for function 2:
mean: 6403.98 mean/area1: 0.986745 mean/area2: 0.986745
standard deviation: 2.06764
coefficient of variation (std/mean): 0.000322868

```

```
area1: 6490 area2: 6490
```

14.4 Comparison under R

The result-files, `ex.res` and `exg2.res`, are compared using the `Rcaliflopp` package under R. We visualize the differences between the 3rd and the 4th values of each line of these files (i.e the pollen and seed integrated flows per m²) that are greater than 1.0e-5, by the R-command:

```
crdiff("ex.res","exg2.res", ival=c(3,4), mdiff=c(1e-5,1e-5))
```

Output are:

```

$V3
      p1 p2    res1    res2    diff
[1,] 66 66 0.942609 0.942581 2.8e-05

```

```
$V4
```

```
      p1 p2  res1    res2    diff
[1,] 66 66 0.9867 0.986745 -4.5e-05
```

Chapter 15

Details about the programme

15.1 The main steps of the programme

The main steps of the programme are shortly sketched here. The user is invited to read this Section for a better understanding of the input, output, warning and error messages.

15.1.1 Preprocessing on the polygons

1. The coordinates are multiplied by `SCALE`¹, a multiple of ten, and then truncated to integers. For example, 2.986 is considered as 2 m if `SCALE= 1`, and as 298 cm if `SCALE= 100`.
2. The landscape is relocated so that the minimal x-coordinate (y-coordinate respect.) is one,
 - when a x-coordinate (y-coordinate respect.), after multiplication by `SCALE`, is greater than `SAFE`¹
 - when it is null or less than zero,
 - systematically when `TRANSLATE`¹ = 1.
3. Simplification of the polygons: the aligned² or too close vertices³, as well as the sharp spikes⁴ are removed from the polygons.
4. The areas and the centroids of the polygons are calculated.
5. Convex subpolygons are created.

15.1.2 Steps for each pair of convex polygons

For each pair of convex polygons (P_1, P_2) , the steps are:

¹`SCALE`, `SAFE`, `DISTP` and `TRANSLATE` are constants set in the file `src/caliconfig.h`.

² When the arccosinus of the angle built by three successive vertices is near to π , the vertices are considered as aligned and the middle one is suppressed.

³ When the distance between two successive vertices is less than or equal to `DISTP`, the second vertex is suppressed.

⁴ When the arccosinus of the angle built by three successive vertices is near to zero, it is supposed that the three vertices draw a sharp spike, and the second one is suppressed.

- When the minimal distance between the polygons P_1 and P_2 is greater than a given threshold, DP⁵, the dispersal function is calculated between the centroids of these polygons, and the result is multiplied by the product of their areas.
- When this distance is greater than the threshold DZ⁵, the dispersal is automatically set to zero.
- Otherwise, for each pair of convex subpolygons in P_1 and P_2 , the **Minkowski sum** is calculated and the flow is estimated by the result of an integration on all the Minkowski sums. The integrand is the product of the individual dispersal function by the area of the intersection between the first subpolygon and a translation of the second one in the pair.

15.1.3 Integration methods

Two integration methods are implemented (See details in Section 4):

- The **grid method** :
Integration is made by discretisation of the **Minkowski sum** on regular grids of points. Several grids of regularly spaced points are generated, each one randomly shifted from the origin. The successive results can be considered as replications.
The iterative process stops when the number of replications is reached.
- The **cubature method**:
This method is a numerical adaptive cubature method over triangles.
The absolute and **relative** precisions can be controlled, as well as the maximal number of evaluations.

15.1.4 Final results

With the grid method, in addition to the **mean of the integrated flow** over the replications, the **coefficient of variation** and the **standard deviation** are calculated.

With the cubature method, in addition to the **integrated flow**, the absolute precision and a **confidence interval** are calculated.

15.2 The individual dispersal functions

In the deliverable, two individual dispersal functions are defined. Others may have been implemented: refer to your installator or see the source code in the file `src/functions.cpp`.

15.2.1 Individual dispersal function of oilseed rape pollen

The first function is the oilseed rape pollen individual dispersal function described by Étienne Klein [KLP+06] until 50 m and by Céline Devaux for distances beyond 50 m [DLAK06]:

$$\phi(t) = \begin{cases} d + er + fr^2 & \text{when } 0 \leq r \leq 1, 5 \\ \frac{b}{1+r^c/a} & \text{when } 50 \leq r < 1, 5 \text{ , } r = \| t \| \\ \left[\frac{b}{1+h^c/a} / (1+h)^g \right] * (1+r)^g & \text{when } r > 50 \end{cases} \quad (15.1)$$

⁵Thresholds are set in the file `src/caliconfig.h`; they are different for each dispersal function. DP constants are the distances beyond which calculation is made between centroids. DZ constants are the distances beyond which dispersal is considered as null.

with $a = 3.80$, $b = 0.03985$, $c = 3.12$, $d = 0.340$, $e = -0.405$, $f = 0.128$, $g = -2.29^6$, $h = 50$ and with t the distance between the source and target points. Distances are in meters. See Fig. 15.1.

For this function, the threshold beyond which the flow is calculated between centroids only, is 100 m.

15.2.2 Individual dispersal function of oilseed rape seeds

The second function is the oilseed rape seed individual dispersal function proposed by Nathalie Colbach [CCDM01b]:

$$\phi(t) = \begin{cases} \frac{b \times c \times r^{(c-2)} \times \exp(-b \times r^c)}{2.0 * \pi} & , \quad r = \|t\|. \end{cases} \quad (15.2)$$

with $b = 1.38930$, $c = 2.08686$ and with t the distance between the source and the target points. Distances are in meter. See Fig. 15.1.

For this function, the threshold beyond which the flow is supposed to be null is 21 m.

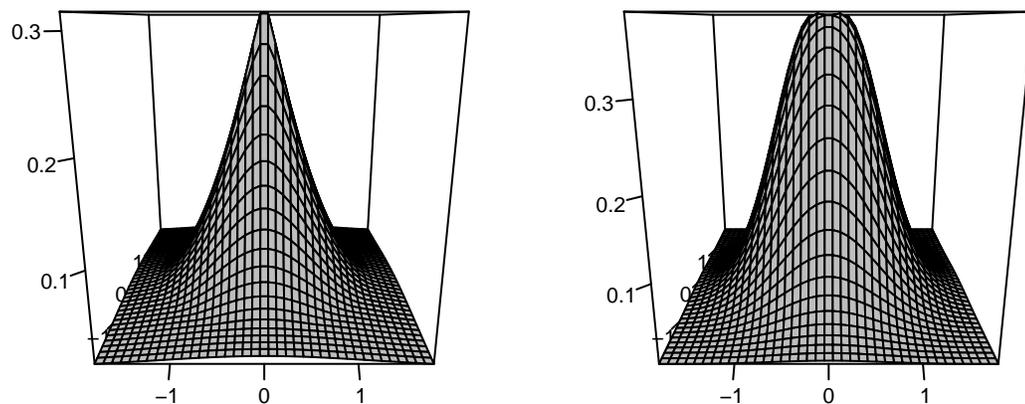


Figure 15.1: Individual Dispersal Function of Pollen (on the left) and Oilseed (on the right) Rape Seeds.

15.2.3 How to modify or add individual dispersal functions

The individual dispersal functions are coded in the C file `src/functions.cpp`. To modify them, change the formulae expressions in the source code. Don't forget they must be smooth functions. Change also the `DP*` and `DZ*` constants in the file `src/caliconfig.h`, i.e the thresholds for calculating dispersal between centroids only and for considering that dispersal is zero, respectively.

⁶According to N. Colbach ([CCDM01a] and [CCDM01b]), g can vary between $-2, 14$ and $-2, 56$.

In the delivered package, up to five dispersal functions can be defined. By default, the `DEFAULT_NFUNCTIONS`⁷ first functions are considered only.

⁷ `DEFAULT_NFUNCTIONS` is defined the file `src/caliconfig.h`.

Chapter 16

Auxiliary Programmes

Additional programmes are provided to compute the polygon areas, the areas of their intersections, and to create files where the polygons are simplified. For these programmes, the format of the polygons-file and its values separator are defined by the constants `INPUT_FORMAT` and `DEFAULT_DELIM`, set in the file `src/caliconfig.h`; they cannot be changed by the user.

On sites where the `Rcaliflopp` or `landm` packages have been installed, some R functions are available in addition to make easier the vizualisation of input and output of `CaliFloPP`.

16.1 Polygon area computation

Usage: `surface -i polygons-filename [-v] [-r result-filename]`

(`surface.exe` instead of `surface` on windows systems).

The option `-v` is for “**verbose**”: it implies output about the decomposition into convex sub-polygons of the non-convex ones.

The results are written on the standard output unit (the screen, by default), or, when the option `-r` is set, on the file it introduces, the structure and content of which are:

1. On the first line, the number of polygons , `npoly`, and the polygons-filename.
2. On each of the `npoly` following lines, two values separated by a tabulate character: the polygon identifier and its area in m^2 .

16.2 Computation of the area of the intersection between two polygons

Usage: `aireintersect -i polygons-filename [-v] [-r result-filename]`

(`aireintersect.exe` instead of `aireintersect` on windows systems).

The option `-v` is for “**verbose**”: it implies output about the decomposition into convex sub-polygons of the non-convex ones.

The areas of non-null intersections are written on the standard output unit, or, when the option `-r` is set, on the file it introduces, the structure and content of which are:

1. On the first line, the number of polygons, `npoly`, and the polygons-filename.

2. On each of the `npoly` following lines, three values separated by a tabulate character: the identifiers of the first and second polygons, and the area of their intersection in m^2 .

Be careful: When a polygon is entirely included in another, the intersection of these two polygons is considered to be null by this programme.

16.3 Polygons simplification

Usage: `polysimplif -i polygons-filename -r result-filename`

(`polysimplif.exe` instead of `polysimplif` on windows systems).

The polygons are simplified: see 3.

The structure and format of the result-file is the same as the structure and format of the input file. The number of decimal digits is determined by `SCALE`, with three decimals at most. The list of the removed vertices is written on the standard error unit.

16.4 R functions

On sites where the `Rcaliflopp` or `landm` packages have been installed, you can use R functions.

To access to the package `Rcaliflopp`,

- if `Rcaliflopp` is installed in the R standard libraries location, type:
`library(Rcaliflopp)`
- if `Rcaliflopp` is installed in a non-standard location, type:
`library(Rcaliflopp, lib.loc='Rcaliflopp-location')`
In this case, you can see the help-files by browsing the file:
`Rcaliflopp-location/Rcaliflopp/html/00Index.html`.

Do the same, to access the package `landm`.

Chapter 17

A Small Glossary

- **$\widehat{\mathcal{F}}$: integrated flow in the cubature method:**
For each pair of convex subpolygons of a given pair of polygons, the **Minkowski sum** is calculated and triangulated. $\widehat{\mathcal{F}}$ is the result of an adaptive cubature integration method on all the triangles.
Special cases: when threshold distances have been set, $\widehat{\mathcal{F}}$ is automatically set to zero, or calculated between centroids only, beyond these distances (see **15.1.2**).
- **$\widehat{\mathcal{F}}$: mean of the integrated flows in the grid method:**
 $\widehat{\mathcal{F}}$ is the sum over all the pairs of convex subpolygons, of the mean of the calculated values over the replications, i.e: $\widehat{\mathcal{F}} = \sum_{i=1}^{i=k} \sum_{j=1}^{j=r} \widehat{f}_{i,j} / r$, where k is the number of pairs of convex subpolygons and $\widehat{f}_{i,j}$ is the calculated integrated flow between one such pair of subpolygons, at the j^{th} grid generation.
Special cases: when threshold distances have been set, $\widehat{\mathcal{F}}$ is automatically set to zero, or calculated between centroids only, beyond these distances (see **15.1.2**).
- **Coefficient of variation in the grid method:**
 $CV = \text{standard deviation} / \text{mean}$.
- **Confidence Interval in the cubature method:**
 $IC = [\widehat{\mathcal{F}} - \text{absolute error}, \widehat{\mathcal{F}} + \text{absolute error}]$
- **Minkowski sum of two polygons A and B .**
This sum is a polygon, denoted by $\dot{A} \oplus B$. It is the set of points p , such that: $p = y - x, x \in A, y \in B$, i.e the set of points covered by B when a vertex of B is moved inside A .
- **Relative error in the cubature method:**
 $\text{relative error} = \text{absolute error} / \text{result}$
- **Standard deviation in the grid method:**
 $\text{standard deviation} = \sqrt{\sum_{j=1}^{j=r} (\widehat{f}_{.j} - \widehat{f}_{..})^2 / (r - 1)}$, where r is the number of replications, i.e the number of grid generations, $\widehat{f}_{.j}$ the result of the grid integration at replication j , and $\widehat{f}_{..}$ the mean result over the j replications.

Part VI

Developer Guide

Chapter 18

Implementation

18.1 Programme steps

The main steps have been described from the user's point of view in Section 15. Here, they are sketched at the programming level.

18.1.1 The main programme and the two pilots

The `main` function is reduced as much as possible, so the developer can easily replace it or insert the package into another one. It decodes the command line and its arguments. When the command has no argument (interactive mode), it calls `califlopp_ad`; when it has arguments (non-interactive mode), it calls `califlopp_sd`.

`califlopp_ad` implements the dialogue with the user while `califlopp_sd` reads the parameter-file. Then, both pilot the preprocessing step before calling the calculation driver.

18.1.2 Preprocessing

Function `ReadPoly`:

1. Read the polygons file and convert the coordinates into integers (->¹`ReadCoord`);
2. Relocate the landscape (-> `TranslatedParcel`);
3. For each polygon:
 - (a) remove aligned vertices and vertices forming a sharp spike;
 - (b) create convex subpolygons: first, determine the essential diagonals, i.e the diagonals which split the polygon into convex parts (-> `Triangulate`), and then determine and store the convex subpolygons ((-> `HMAlgor`);
 - (c) compute areas (-> `Area2`).

18.1.3 Calculation steps

The function `suite` pilots the calculations process. It realizes the following tasks:

1. Create an object, `methode`, of class `methodGrid` or `methodAdapt`.

¹Arrow is for a call to a subroutine.

2. Call its method `VerifArgu` to verify its attributes.
3. Pilot the loop on the required pairs of polygons: for each of them, call the function `go` which invokes the methods `CalcR` on `methode` to perform the calculations, `Print` to output the results on the screen, and `PrintFic` to output them on a result-file.

18.1.4 Calculation by the grid method

The method `CalcR` of the class `methodGrid` is summarized by the following algorithm:
(The names of the devoted functions are between square brackets.)

Algorithm 7: `methodGrid::CalcR`

Data: A pair of polygons A and B , nf individual dispersal functions, user-defined parameters.

Result: Dispersal estimations from A to B by the grid method.

- 1 Calculation of *mindist*, the minimal distance between the polygons.
- 2 **foreach** *dispersal function* ϕ **do**
- 3 **if** *mindist* \geq *threshold for function annulment* **then**
- 4 *result* = 0
- 5 **end**
- 6 **if** *mindist* \geq *threshold for calculation between centroids* **then**
- 7 *t* = distance between centroids; *result* = $\phi(t) \times \text{area}(A) \times \text{area}(B)$
- 8 **end**
- 9 **end**
- // In the other cases: one function at least should be integrated
- 10 **foreach** *pair of convex subpolygons* A_i and B_j in A and B **do**
- 11 Compute and store their Minkowski sum: *sommeM_{ij}* [SommeMinkowski];
- 12 **end**
- 13 **foreach** *replication* **do**
- 14 **foreach** *pair of convex subpolygons* A_i and B_j **do**
- 15 Grid generation [Integration]:
- 16 **foreach** *point* t of the grid **do**
- 17 **if** $t \in \text{sommeM}_{ij}$ [InPolyConvex] **then**
- 18 $ar = \text{area}(A_i \cap (B_j - t))$; [ConvexIntersect]
- 19 **foreach** *dispersal function* ϕ to be integrated **do**
- 20 *result* += $\phi(t) \times ar$;
- 21 **end**
- 22 **end**
- 23 **end**
- 24 **end**
- 25 **end**
- 26 Compute the final results: means over the replications, standard deviation.

18.1.5 Calculation by the cubature method

The algorithm 8 summarizes the tasks realized by the method `CalcR` of the `methodAdapt` class (the names of the devoted functions are between square brackets).

$octo_\phi$ stands for the smallest octogon centered in $(0,0)$ which includes the circle of radius equal to the distance beyond which the dispersal function ϕ becomes nul; $octo_\phi$ is an attribute of the `methodAdapt` class and is created by the class constructor.

Algorithm 8: `methodAdapt::CalcR`

```

Data: A pair of polygons  $A$  and  $B$ ,  $nf$  individual dispersal functions, user-defined
parameters.
Result: Dispersal estimations from  $A$  to  $B$  by the cubature method.
1 Calculation of mindist, the minimal distance between the polygons.
2 foreach dispersal function  $\phi$  do
3   if mindist  $\geq$  threshold for function annulment then
4     result = 0
5   end
6   if mindist  $\geq$  threshold for calculation between centroids then
7      $t$  = distance between centroids; result =  $\phi(t) \times \text{area}(A) \times \text{area}(B)$ 
8   end
9   // In the other cases: integration should be done
10  stvertce =  $\emptyset$ ; result = 0;
11  foreach pair of convex subpolygons  $A_i$  and  $B_j$  of  $A$  and  $B$  do
12    Compute and store the Minkowski sum: sommeMij; [ SommeMinkowski]
13    if dispersal has no limit then
14       $S$  = sommeMij;
15    else
16      // no dispersal beyond a given distance
17       $S$  = sommeMij  $\cap$   $octo_\phi$  [ TConvexIntersect];
18    end
19    if  $S \neq \emptyset$  then
20      if  $(0,0) \in S$  [ InPolyConvex] then
21        stvertce+ = triangulation of  $S$  from  $(0,0)$  [ Triangulate0];
22      else
23        stvertce+ = triangulation of  $S$  from any vertex [ Triangulate];
24      end
25    end
26  end
27  // End of the loop over  $A_i, B_j$ 
28  Integration on the stvertce triangles for function  $\phi$  [ Adapt::Integration];
29 end
30 // End of the loop over the functions

```

18.2 Data structures

The main data structures are described in the following array:

Name	Dimension	Type	Content
Poly	npoly, nspoly, nvert, DIM	tPolygoni (integer)	Polygons coordinates, counterclockwise sorted, non-closed polygons
ni	npoly, nspoly	integer	$ni_{i,j}$: number of vertices in the sub-polygon j of the polygon i
a	npoly	integer	a_i : number of convex subpolygons of the polygon i
vertices	structure	tVertex (integer)	Linked list of the ordered vertices of a polygon. Each element contains:
	V[DIM]	integer	- coordinates of a vertex,
	next		- pointer to the next vertex or to the head of the list if none,
	prev		- pointer to the preceding vertex or to the head of the list if none,
vnum	integer	- vertex indices	
sommeM	nvert, DIM	tPolygoni (integer)	Minkowski Sum
intersection	id. as vertices	tdVertex (real)	Intersection of polygons

npoly: number of polygons

nspoly: number of convex subpolygons in a polygon

nvert: number of vertices in a polygon

DIM: space dimension (here =2).

18.3 Functions list

The functions used for integration by the cubature method are methods of the class `Adapt`; they are coded in the files of the directory `src/adapt`. The other main functions are summarized by the following list:

(Words in *italic* refer to data structures.)

Function name	File name	Fonction
main	main.cpp	Decode the command line
ecrmess	util.cpp	Error message output and return to the calling programme
libMem	util.cpp	Memory de-allocation
califlopp_ad	fluxad.cpp	Pilot the interactive mode
califlopp_sd	fluxsd.cpp	Pilot the non-interactive mode
suite	go.cpp	Pilot the loop over the pairs of polygons
go	go.cpp	Pilot the treatment of one pair of polygons
read1Poly, read2Poly	read1Poly.cpp	Read the coordinates in format 1 and 2, resp.
ReadCoord	readPoly.cpp	Read the polygons-file; verify the coordinates; scale multiplication of the coordinates
ReadVertices	readPoly.cpp	Create <i>vertices</i>
ReadPoly	readPoly.cpp	Create <i>Poly</i> with: - aligned vertices removal - non-convex polygons splitting - areas computation
TranslateParcel	readPoly.cpp	Relocation of the polygons
ConvexIntersect	intersection.cpp	Convexity test and creation of <i>intersection</i>
Triangulate, HMAlgor, Area2	geom.cpp	Programmes of geometric computation
SommeMinkowski	zoneintegration.cpp	Compute <i>sommeM</i>
genrand_real2	mt19937ar.cpp	Random numbers generation ¹
f0,f1,fX	functions.cpp	Individual dispersal functions
f_	methodAdapt.cpp	The integrand for cubature method
Integration	methodGrid.cpp, methodAdapt.cpp	Integration
CalcR	methodGrid.cpp, methodAdapt.cpp	Compute one result
Print, PrintFic	methodGrid.cpp, methodAdapt.cpp	Output results on screen and on file, resp.

See reference [\[MN98\]](#).

Error codes: The list and meaning of the errors codes can be found in the file `calierror.h`.

Chapter 19

How to Modify

It may be useful to know how to modify some parts. Among them:

- The individual dispersal functions: see Section [15.2.3](#).
- The format of the polygons-file: see the files `read1Poly.cpp` and `read2Poly.cpp`.
- In interactive mode, the dialogue with the user: see the file `fluxad.cpp`, and the `ReadArgu` method in the files `methodGrid.cpp` and `methodAdapt.cpp`.
- Screen output: see the file `go.cpp`, and the `Print` method in the files `methodGrid.cpp` and `methodAdapt.cpp`.
- File output: output on the result-file depend on the constant `OUTPUT_FORMAT` set in the file `caliconfig.h`. They are carried on by the `suite` function and by the `PrintFic` methods in the files `methodGrid.cpp` and `methodAdapt.cpp`.
- Erroneous polygons treatment: the identifiers of the erroneous polygons are made negative by the `ReadPoly` function. Their treatment depends on the constant `ERR_POLY` set in the file `caliconfig.h`.
- Memory allocation: memory allocation is made via the macros `CREER` and `NEW` and de-allocation via the macros `DETRU` and `FREE`; they are coded in the file `calimacros.h`.
- Random number generator: see the variable `COPTIONS2` in the file `obj/subdir.mk` and the corresponding code in `methodGrid.cpp`.
- Computing time measurement: see the file `timing.cpp`.
- Estimation of several integrals by the cubature method: this possibility can be added when several integrals have enough similarity. Estimation of all of them can be made in one call. It is less time consuming. For that, modify:
 - the function `f_` in the file `methodAdapt.cpp`: the vector `funvls` should contain as many results as integrals on output.
 - the function `CalcR` in the file `methodAdapt.cpp`: the first argument of the `Adapt` constructor should be equal to the number of integrals.
 - the output operator in the file `adapt/Adapt.h`: it should print as many results and absolute errors as integrals.

Part VII
Bibliography

Bibliography

- [BE92] Jarle Berntsen and Terje O. Espelid. Algorithm 706, DCUTRI: An algorithm for adaptative cubature over a collection of triangles. *ACM Transactions on Mathematical Software*, 18(3):329–342, 1992. **23, 25**
- [CCDM01a] N. Colbach, C. Clermont-Dauphin, and J.M. Meynard. Genesys: a model of the influence of cropping system on gene escape from herbicide tolerant rapeseed crops to rape volunteers. i. temporal evolution of a population of rapeseed volunteers in a field. *Agriculture, Ecosystems and Environnement*, 83:235–253, 2001. **1, 9, 79**
- [CCDM01b] N. Colbach, C. Clermont-Dauphin, and J.M. Meynard. Genesys: a model of the influence of cropping system on gene escape from herbicide tolerant rapeseed crops to rape volunteers. ii. genetic exchanges among volunteer and cropped populations in a small region. *Agriculture, Ecosystems and Environnement*, 83:255–270, 2001. **1, 9, 79**
- [CRA] CRAN. R: a free software environment for statistical computing and graphics. URL: <http://www.r-project.org/>. **47**
- [DLAK06] C. Devaux, C. Lavigne, F. Austerlitz, and E.K. Klein. Modelling and estimating pollen movement in oilseed rape (*Brassica napus*) at the landscape scale using genetic markers. *Molecular Ecology*, 2006. **78**
- [KLP⁺06] E.K. Klein, C. Lavigne, H. Picault, M. Renard, and P.H. Gouyon. Pollen dispersal of oilseed rape: estimation of the dispersal function and effects of field dimensions. *Applied Ecology*, 43:1141–1151, 2006. **78**
- [LKV⁺98] C. Lavigne, E.K. Klein, P. Vallée, J. Pierre, B. Godelle, and M. Renard. A pollen-dispersal experiment with transgenic oilseed rape. estimation of the average pollen dispersal of an individual plant within a field. *Theoretical and Applied Genetics*, 96:886–896, 1998. **9**
- [MN98] M. Matsumoto and T. Nishimura. Mersenne twister: A 623-dimensionally equidistributed uniform pseudo-random number generator. *ACM Transactions on Modeling and Computer Simulation*, 8(1):3–30, 1998. **91**
- [NAG] *The NAG Fortran Library*.
URL: <http://nag.co.uk/numeric/fl/FLdescription.asp>. **16**
- [O’R98] Joseph O’Rourke. *Computational Geometry in C*. Cambridge University Press, second edition edition, 1998. Supplementary material <http://maven.smith.edu/~orourke/books/compgeom.html>. **17, 19, 21**
- [Y.05] Fu Y. Méthodes d’intégration pour le calcul des flux de gènes entre parcelles dans un paysage agricole. Master’s thesis, École Centrale de Nantes, 2005. Mémoire de stage, Unité INRA MIA, Jouy-en-Josas. **3**

The red figures at the end of each reference refers to the pages in the document.