# QUASIMONT

QUAdrature of SINgular polynomials using a MONonomial Transformation rule

# USER MANUAL





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Chapter

# **PRELIMINARIES**

This user manual provides a detailed description of the functionalities, correct installation and usage of the open-source C++ library QUASIMONT. Users of the library can refer to the following content for setting and executing the code within as well as integrating it in their custom application. The principles behind its implementations are discussed in the this first chapter, followed by instructions for correctly building and running the library in a Linux distribution (outlined in the second and third chapter). The a concluding chapter describes its inner workings and implementation. Being a mathematical software, a solid grasp of various topics in mathematical and numerical analysis is an advantage for the user to exploit the library to its fullest capability. In the second section of this chapter we provide a brief coverage on some of those concepts such as interpolatory quadrature formulae, Gaussian quadrature and asymptotic error estimation which are required for users that are not familiar with the aforementioned topics. This overview is far from complete and self-contained, and we direct to [8, 9], and references therein, as the primary sources for a thorough theoretical exposition on the mathematical foundations of QUASIMONT.

#### 1.1 OVERVIEW

As the name suggests, QUASIMONT provides a framework for the high-precision numerical computation of singular (definite) integrals whose integrands are generalised polynomials whose monomial terms have a non-integer degree. First and foremost one has to understand the motivation for such library to exist, in order to effectively decide whether or not its usage is necessary for her/his own needs. Different techniques have been proposed to numerically approximate singular and hyper-singular integrals however the accuracy of their performances is limited by their computational cost, effectively reducing the implementation and application of those to a classical polynomials. We wrote QUASIMONT with the aim of helping the user when both generalized singular polynomials and high precision quadrature are required (examples are outlined in the opening section of [9]) while at the same time avoiding the compromising between accuracy and time of execution. The algorithm that stands at the core of the library is based on error estimation for Gauss-Legendre (G-L) quadrature applied to monomials of non-integer degree and on the processing of the parameters of integration (discussed in the following section) through an ad-hoc numerical manipulation that depends on the characteristics of the generalised polynomial to be integrated. This method, is based also on the application of an optimized monomial transformation rule, the background theory of which is reported in [8] while the algorithm paper in [9] reports its automatised implementation with related library. The monomial quadrature rule is a result of a novel exact asymptotic error estimate for the G-L quadrature formula introduced in [8] that shows in depth the potentialities of GL quadrature to integrate generalized polynomials composed by monomials of non-integer degree. Specifically it shows the degree of precision of the quadrature rule for singular definite integrals constituted of generalized polynomials with a target relative error (see IEEE floating-point formats' machine-epsilon in Table 1.1). In particular it extends the range of validity of the rule to polynomials of non-integer degree and in particular to those characterised by an end-point singularity in the integration interval. We want to emphasize these features of QUASIMONT right at the start of this user manual so that the user has a clearer understanding of the contexts in which it becomes necessary. In fact, as we will show

in the test drivers section (see Section 2.4), QUASIMONT significantly outperforms classical G-L quadrature for polynomials whose exponents' sequence is composed of either rational or irrational numbers (henceforth referred to as **Müntz sequence**, see Subsection 1.2.4). To consistently reach such performance the following steps are followed (see the following Chapter):

- 1. select a fixed threshold for the remainder of the integration rule (e.g. the machine-epsilon in IEEE double precision);
- 2. exploit the in-depth error estimation of the G-L quadrature;
- 3. design a monomial transformation to obtain the selected precision for the quadrature of a specified family of generalized polynomials.

Floating-point formats				
Common name (official)	single (binary32)	double (binary64)	quadruple (binary128)	
n. bits	32	64	128	
n. decimal digits	7	16	34	
epsilon	1.1921 e-07	2.2204 e-16	1.9259 e-34	
real min	1.1755 e-38	2.2251 e-308	3.362 e-4932	
real max	$3.4028 \text{ e}{+38}$	1.7977  e + 308	1.190  e + 4932	

Table 1.1: Some parameters of the most common floating-point formats specified by the IEEE 754 standard

The increased performance w.r.t. classical G-L quadrature is measured as a higher precision of the resulting integral as well as a fewer number of quadrature nodes and weights amounting to cheaper computational cost required at run-time by any application. On the other hand, whilst QUASIMONT allows for the integration of monomials and polynomials of integer degree, we remark that these integrands are not the cases for which the library was written nor its execution is necessary to achieve accurate results (interpolatory classical and generalised Gaussian rules will suffice). QUASIMONT is entirely written in C++17; beside the speed and versatility of the language, the primary motivation behind such choice was the accessibility to other open-source packages (see Section 2.1) that were essential for the implementation of different routines that extract fundamental information for the precise quadrature of singular integrals. One such example is the ability of handling operations in higher-than-double floating-point arithmetic (e.g. IEEE quadruple floating-point format or higher, see Table 1.1), provided in the GMP - GNU Multi Precision library, without which the precise computation of the quadrature parameters and the quadrature itself would have not been possible. Due to its relatively small scope, QUASIMONT is not object-oriented; instead all its functionalities are implemented in different functions interacting through the quasimont module (see Section 2.1 and 2.2).

#### 1.2 MATHEMATICAL BACKGROUND

Given a map  $f:[a,b]\to\mathbb{R}$  its definite integral is defined as the linear operator

$$I(f) := \int_{a}^{b} f(x)dx, \quad \mathcal{I} := [a, b] \subset \mathbb{R}$$
(1.1)

The driving purpose of QUASIMONT is to compute a precise numerical approximation of I(f) with polynomial functions i.e. when  $f \in \mathbb{P}_{\alpha}[x]$ . Usually, polynomials are characterised by a natural degree  $k \in \mathbb{Z}$  however our library extends it to the a sub-space of the polynomials of non-integer (real) degree  $\alpha \in (-1, +\infty)$ . Of course the analytic integration of polynomial functions is trivial, always leading to an exact form (polynomial) of the primitive function  $\tilde{f}$  to be evaluated on the real bounds of integration

$$I(f) = \left[\tilde{f}(x)\right]_{x=a}^{x=b}, \quad \tilde{f} \in \mathbb{P}_{k+1}[x] \ \forall f \in \mathbb{P}_k[x]$$

$$(1.2)$$

There are applications however, in particular in numerical methods in various computational sciences and engineering, where such polynomials are not explicitly defined but instead they model the behavior of a computed physical quantity (e.g. source integrals in the Boundary Element Method). In scientific computing it is also frequently encountered the further constraint of integrating functions that feature an endpoint singularity in either or both the bounds of integration, which cannot be represented exactly with regular high-order polynomials.

#### 1.2.1 INTERPOLATORY QUADRATURE

We let  $f: \mathcal{I} = [a,b] \to \mathbb{R}$  be any function; we want to compute I(f) although unfortunately its primitive is not known. One solution is to substitute the function with a polynomial interpolating some of its values at sampled point, called **nodes**. Such nodes constitute a finite, countable set  $\mathcal{I}_h := \{x_0, x_1, \ldots, x_{n-1}, x_n\}$  which can be thought as a discretisation of the original domain of integration  $\mathcal{I}$ . The cardinality of such set is n+1 and it is linked with the degree of the polynomial interpolating f(x); in particular such degree will be n = (n+1) - 1. The interpolating polynomial  $\mathbb{P}_n \ni \mathcal{L}_n(x) := \sum_{j=0}^n \ell_j(x) f(x_j)$  is expressed in the so-called **Lagrangian basis** whose generators  $\ell_j(x) \in \mathbb{P}_n$ . We will not address the theoretical aspects of Lagrangian interpolation and approximation theory although the user may refer to [9] and references therein for further details. We can now express the kernel through an arbitrary precise approximating polynomial of degree n

$$f(x) = \mathcal{L}_n(x) + R_n(f) = \sum_{j=0}^n \ell_j(x) f(x_j) + R_n(f) \quad x_j \in \mathcal{I}_h, \ \forall j = 0, ..., n$$
(1.3)

By substituting (1.3) in (1.1) we obtain an approximation of the initial integral known as an **interpolatory** quadrature

$$I(f) = \int_{a}^{b} (\mathcal{L}_{n}(x) + R_{n}(f)) dx = \sum_{j=0}^{n} f(x_{j}) \int_{a}^{b} \ell_{j}(x) dx + \int_{a}^{b} R_{n}(x) = \sum_{j=0}^{n} w_{j} f(x_{j}) + E_{n}(f)$$
(1.4)

where we defined the **weights**  $w_j$  of the quadrature formula as the integral of the Lagrangian basis generators and the **remainder** or **error** as  $E_n(f) := \int_a^b R_n(f) dx$ . It is a well known result in numerical analysis that interpolatory quadrature rules are exact, i.e.  $R_n(f) = 0$  if the kernel is a polynomial of degree up to n.

#### 1.2.2 GAUSSIAN QUADRATURE FORMULAE

One issue with numerical integration using interpolatory quadrature is the choice of the distribution of the nodes. The simplest case is of course that of a uniformly distributed partition  $\mathcal{I}_h = \left\{x_j = a + (j-1)h, h := \frac{b-a}{n}\right\}_{j=0,1,\dots,n}$  which results in what is known as a **Newton-Cotes formula**. There are however better choices for the nodes distribution depending on the properties and behaviour of f(x) in  $\mathcal{I}$ ; in particular a **Gaussian quadrature formula** is one where each of the nodes correspond to the root of an orthogonal polynomial. To introduce these approximations we now let the integrand to be an arbitrarily regular function

$$C^{m}[\mathcal{I}] \ni f(x) = w(x)g(x), \quad m \in \mathbb{N}$$
(1.5)

where the factorised g(x) always contains its most regular part whereas w(x), known as the **weight function** contains, if present, any irregular and/or singular part of f(x). Now if the weight function is not null everywhere in  $\mathcal{I}$  and we can find a sequence of classical polynomials  $P := \{p_j(x) \in \mathbb{P}_j\}_{j=0,1,\dots}$  s.t.

$$\int_{a}^{b} w(x)p_{j}(x)p_{k}(x) dx = \alpha_{jk}\delta_{jk}, \quad \forall p_{j}, \ p_{k} \in P$$

$$(1.6)$$

where  $\delta_{jk}$  is the Kronecker delta, then P represents of a system of orthogonal polynomials w.r.t. w(x). Any Gaussian quadrature formula is exact for any classical polynomial integrand of degree up to 2n-1, where n is the number of the nodes in the partition  $\mathcal{I}_h$ . It is therefore easy to see why Gaussian quadrature is normally preferred over Newton-Cotes formulae for the numerical integration of both regular functions, of which classical and generalised polynomials are a subset of particular relevance and interest in mathematical modelling, and irregular or singular integrands on which QUASIMONT is focused. Arguably the most famous, surely one of the most widely used, Gaussian quadrature rule is the G-L formula (mentioned in the opening Section 1.1). With the G-L quadrature rule the sequence P is made of Legendre's polynomials which are orthogonal to the constant weight function w(x) = 1 in the symmetric integration interval  $\mathcal{I} = [a = -1, b = +1]$ .

#### 1.2.3 ASYMPTOTIC ERROR ESTIMATION

We now ask ourselves how accurate a G-L quadrature formula with n nodes really is. Obviously if  $f(x) \in \mathbb{P}_k$ ,  $k \in \mathbb{N}$  we have an exact answer to this question i.e. if  $k \leq 2n-1$  then  $E_n(f)=0$  as explained in the section above. On the other hand if  $k \geq 2n-1$ , we can resort to an **a-posteriori error estimation** using 1.2 as

$$E_n(f) = \frac{|I(f) - I_h(f)|}{|I(f)|}, \quad I_h(f) := \sum_{j=0}^n w_j f(x_j)$$
(1.7)

where the sequence of pairs  $\{(x_j, w_j)\}_{j=0,...,n}$  is the set of nodes and weights of the G-L quadrature rule. However there are many instances, in any development and design process, in which the primitive of the integrand either has no closed form or is too computationally expensive to be determined and evaluated. In those cases an **a-priori error estimation** is needed (see Sub-section 3.3 in [9] and cited references), which are often obtained via asymptotic analysis, meaning that their evaluation is precise when  $n \to +\infty$ . In [8], one of the author of the present user manual, derived an improved, closed form, a-priori error estimation for a G-L formula, namely

$$E_n(f) = -2^{-2\lambda} \lambda \left( \frac{B(2\lambda, 2n - \lambda)}{2n + \lambda} - \frac{B(2\lambda, 2 + 2n - \lambda)}{2 + 2n + \lambda} \right)$$

$$\tag{1.8}$$

where  $B(z,w) := \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}$  is the Euler's Beta function. This result proved to be of paramount importance for the development of an ad-hoc quadrature rule whose error can be computed a-priori for any possible integrand function. In particular, given a specified number of quadrature nodes n, the fast evaluation of the above estimates for several non-integer values of  $\lambda \in (-1, \lambda_{\text{max}})$ , depicted in Figure 1.1 allows to determine, with arbitrary precision, the upper and lower bounds of the exponent s.t. the error estimate is accurate within a pre-determined finite-arithmetic threshold (that we specified to be the machine-epsilon in double f.p. format).

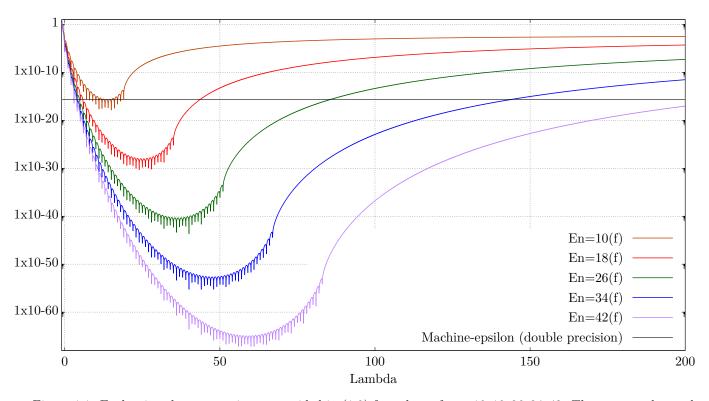


Figure 1.1: Evaluation the error estimate provided in (1.8) for values of n = 10, 18, 26, 34, 42. The pattern observed is that, while the estimates display a polynomial decay that varies negligibly with n, the growth for  $\lambda > d = 2n - 1$  of the G-L formula is quasi-logarithmic which causes the variation of  $\beta_{\text{max}}$  with n to be significant. It can be deduced that estimate (1.8) provides an exact representation of the actual asymptotic behaviour of the remainder of a G-L quadrature formula that can be implemented in finite-arithmetic by setting a pre-determined exactness threshold. We also note that for n = 10 the estimate barely reaches the machine-epsilon threshold entailing that it is the minimum number of nodes that can be used to achieve double precision quadrature. This plot has been realised using the secondary module of QUASIMONT (see Section 3.4).

By identifying this interval of finite-arithmetic equivalent exactness with the aforementioned bounds  $[\beta_{\min}, \beta_{\max}]$  then clearly (1.8) enables the design of a specific transformation based on the ad-hoc processing on the characteristics of the generalized polynomial to be integrated and on the performance of the G-L quadrature in terms of relative error estimate (see Sub-section 1.2.5).

#### 1.2.4 MÜNTZ THEOREM AND SINGULAR POLYNOMIALS

In the opening digression of the Section we mentioned that QUASIMONT extends the integration of generalised polynomials of non-integer degree in the range  $(-1, +\infty)$ . As the reader will find in [8] and references therein, a complete theory on the properties of these kind of functions relates to Muntz polynomials, orthogonal Müntz polynomials and their numerical computation. We assume that the generalized polynomials features a sequence of (real) exponents that is a subset of a Müntz sequence, i.e. a sequence of real, non-negative numbers  $\Lambda := \{\lambda_j > \lambda_{j-1}, \ \lambda_0 > -1\}$  s.t.

$$\sum_{j=0}^{+\infty} \frac{1}{\lambda_j} = +\infty \tag{1.9}$$

Such condition satisfies the known **Müntz theorem** for which the vector space  $\Pi(\Lambda) := \operatorname{span}\{x^{\lambda_j}\}$  spanned by the monomials of degree in  $\Lambda$  is dense in  $\mathcal{C}(0,1]$ . Elements  $p^{(m)}(x) = \sum_{j=0}^r c_j \, x^{\lambda_j} \in \Pi(\Lambda)$  are therefore known as Müntz polynomials of degree  $\lambda_r$  defined in (0,1]. In the following we shall assume that a polynomial with r+1 terms having at least one constituting monomial of non-integer degree that are a subset of  $\Lambda$  are to be considered Müntz polynomials. Our library is capable of approximating the integral of generalised polynomials with a strong endpoint singularity in [0,1] (intended as a subset of Müntz polynomials) with an arbitrary fixed precision (e.g. the a-posteriori remainder falls below the machine-epsilon value in double f.p. format) combining G-L quadrature to an ad-hoc designed monomial transformation rule.

#### 1.2.5 INTEGRATION INTERVAL

The fundamental idea behind the monomial quadrature rule is to use a **monomial map** of the unitary interval [0,1] (over which Müntz polynomials are defined) onto itself to transform the nodes (and thus the weights) of the G-L quadrature and allow high precision numerical integration of generalised polynomials that potentially feature endpoint singularities. For this purpose we need to introduce the **affine map** to map a standard G-L quadrature rule, defined in [-1,1] onto a generic interval I=[a,b] and in particular to our case of interest [a=0,b=1]. Introducing a (linear) affine map  $\varphi:[-1,1] \to [a,b]$  specified as

$$\varphi(\tilde{x}) := \alpha \, \tilde{x} + \beta \tag{1.10}$$

associated to any G-L (or any Gaussian formula, really) quadrature rule in I = [a, b]. It is easy to see that  $\varphi(\tilde{x} = -1) = \beta - \alpha \equiv a$  and  $\varphi(\tilde{x} = +1) = \alpha - \beta \equiv b$ . As such (1.1) becomes

$$I(f) = \int_{a}^{b} f(x)dx = J_{[a,b]} \int_{-1}^{+1} f\left(\frac{b-a}{2}\tilde{x} + \frac{a+b}{2}\right) d\tilde{x}, \quad J_{[a,b]} := \frac{b-a}{2}$$
(1.11)

This new form (1.11) of the integral can now be computed numerically using the G-L quadrature rule; for our case of [a = 0, b = 1] it will become

$$I(f) = \frac{1}{2} \int_{-1}^{+1} f\left(\frac{1}{2}\tilde{x} + \frac{1}{2}\right) d\tilde{x}$$
 (1.12)

where  $f\left(\frac{1}{2}\tilde{x} + \frac{1}{2}\right) = \sum_{j=0}^{r} c_j \left(\frac{1}{2}\tilde{x} + \frac{1}{2}\right)^{\lambda_j} \in \Pi(\Lambda)$  is an affinely mapped Müntz polynomial.

#### 1.2.6 MONOMIAL TRANSFORMATION

We refer the user to [8, 9] for detailed insights regarding this topic, however we outline the basic ingredients of the recipe. Given a (input) Müntz polynomial we define  $\lambda_{\min}$  and  $\lambda_{\max}$  as the smallest and greatest values in the Müntz sequence of exponents. With reference to Sub-section 1.2.4 we know that  $\lambda_{\min} > -1$  (we consider integrable functions) and we make reference to  $\lambda_{\max}$  as the degree of the polynomial. We recall that only with classical polynomials (for which  $\lambda_j \in \mathbb{N}$ ) the G-L quadrature rule with at least  $n = \frac{\lambda_{\max} + 1}{2}$  nodes i.e. with  $E_n(f) = 0$ . Unfortunately in finite arithmetic computing such exact result can never be achieved, and it is limited to the machine-epsilon f.p. format that is specified. Ragardless of sucg precision, generalised singular polynomials, s.a. those in Müntz vector space, will be integrated with low accuracy by classical G-L quadrature with the prescribed number of nodes n. The study of estimate (1.8) allows to construct the parameters necessary to compute a monomial transformation  $\gamma(\tilde{x})$ :  $[0,1] \rightarrow [0,1]$ , for the set of polynomials uniquely identified with  $\lambda_{\min}$  and  $\lambda_{\max}$ , defined as

$$x = \gamma(\tilde{x}) = \tilde{x}^r, \quad \tilde{x} = (1.10) \tag{1.13}$$

with the constraint

$$\frac{1 + \beta_{\min}(n)}{1 + \lambda_{\min}} < r < \frac{1 + \beta_{\max}(n)}{1 + \lambda_{\max}} \tag{1.14}$$

where  $\beta_{\min}(n)$  and  $\beta_{\max}(n)$  are the minimum and maximum exponents that can be integrated with a relative error that is strictly lower than a fixed target floating-point finite precision as computed with (1.8). For each pair of  $(\beta_{\min}(n), \beta_{\max}(n))$  there exist a unique minimum value of n that satisfy the above constraint and it is proved [8] to coincide with the only real root of this 7<sup>th</sup> degree polynomial

$$(-4.0693 \cdot 10^{-3} + 4.1296 \cdot 10^{-4})[(8.8147 + 1.0123 \cdot 10^{-1}n^{2}) \cdot (1 + \lambda_{\min}) - (1 + \lambda_{\max})^{3}] - (1 + \lambda_{\max})^{3}$$
(1.15)

Once all these parameters are computed, one can easily compute r, for example, as a linear interpolation between the two constraints in (1.14) and easily derive the new nodes of the G-L formula with (1.13) which we relabelled as the original, pre-affine map, nodes for simplicity. Whence the optimal new distribution of G-L nodes is obtained by the map, the new weights are computed as well accordingly [8, 9] as

$$w_j = r\tilde{x}_j^{r-1}\tilde{w}_j \quad \forall j = 0, ..., n \tag{1.16}$$

where  $\tilde{x}_j$ ,  $\tilde{w}_j$  are the classical G-L nodes and weights respectively, being mapped in [0,1] by  $\tilde{\varphi}$ . This new configuration of the G-L quadrature parameters is optimal w.r.t. the singular behaviour of a generalise polynomial of non-integer degree near one or both bounds of the integration interval.

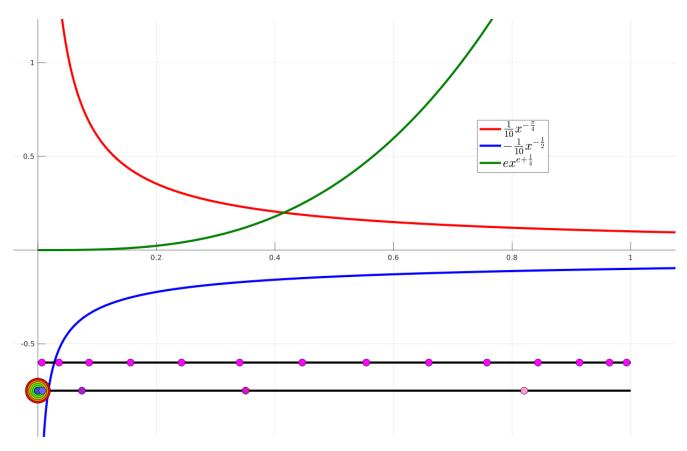


Figure 1.2: This plot shows three singular monomial terms of a Müntz polynomial above. On the bottom of the graph there is the distribution in [0,1] of the n=14 nodes of the classical G-L formula (in magenta) and, further below, the new nodes obtained by the monomial quadrature rule (in linear color gradient). Due to the extreme clustering around the infiumum, the latter are progressively scaled down in dimension from a=0 to b=1. We can clearly see that the linear action of the affine map (1.10) does not stretch the distribution of the classical G-L nodes which therefore preserve in [0,1] the symmetric property they featured in [-1,1]; visually an insufficient number of nodes  $\tilde{x}$  are placed closed to the endpoints of [0,1] where the singularity is, causing a consistent loss in accuracy for the respective quadrature rule. On the other hand, the action of an ad-hoc monomial map (1.13) to the nodes (whose order r=28.77 is given by (1.14) for the present case) will cluster the vast majority of them around the endpoint singularities of  $x^{-\frac{\pi}{4}}$  and  $x^{-\frac{1}{2}}$ .

Considering an instance of such Müntz polynomial

$$\Pi(\Lambda)\ni p(x)=ex^{e+\frac{1}{4}}-\frac{1}{10}x^{-\frac{1}{2}}+\frac{1}{10}x^{-\frac{\pi}{4}}\,,\quad \Lambda=\left\{\,-\frac{\pi}{4},-\frac{1}{2},e+\frac{1}{3}\right\}$$

a visual representation is reported in Figure 1.2 on the effect that an ad-hoc designed monomial map has on the asymetric redistribution of the G-L quadrature parameters which are listed in Table 1.2 for reference.

	Classical G-L parameters		New G-L parameters	
$j \in \mathbb{N}$	$x_j \in [0,1]$	$w_j \in \mathbb{R}^+$	$x_j \in [0, 1]$	$w_j \in \mathbb{R}^+$
0	0.00685809565159384	0.0175597301658759	5.58247922741512e-63	4.11231619931278e-61
1	0.0357825581682132	0.0400790435798801	2.44695140063495e-42	7.88526679349951e-41
2	0.0863993424651175	0.0607592853439516	$2.52951532315787\mathrm{e}\text{-}31$	5.11781542764354e-30
3	0.156353547594157	0.0786015835790968	6.51929796325047e-24	9.42908328714637e-23
4	0.242375681820923	0.0927691987389689	1.95675667095192e-18	2.15474891008643e-17
5	0.340443815536055	0.102599231860648	3.44180025480158e-14	2.98421017862521e-13
6	0.445972525646328	0.107631926731579	8.13715952769522e-11	5.65003223119147e-10
7	0.554027474353672	0.107631926731579	4.18125660540031e-08	2.33701617760019e-07
8	0.659556184463945	0.102599231860648	6.30683776156361e-06	2.82259817558914e-05
9	0.757624318179077	0.0927691987389689	0.000340288421120315	0.00119878736245905
10	0.843646452405843	0.0786015835790968	0.00750950989496675	0.0201292451904070
11	0.913600657534883	0.0607592853439516	0.0742930434150393	0.142150858859985
12	0.964217441831787	0.0400790435798801	0.350516762468882	0.419175839329777
13	0.993141904348406	0.0175597301658759	0.820378484398468	0.417316809008697

Table 1.2: List of all the n = 14 G-L nodes and weights before (classical) and after the monomial transformation of order r = 28.77 depicted in Figure 1.2.

#### 1.3 ACKNOWLEDGEMENTS

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# INSTALLATION

In the following chapter we illustrate how to build executable files with QUASIMONT from its source code as well as the dependencies needed at link-time by the resulting application. We begin from the latter issue by outlining the third-party source code necessary for the library prior to the compilation itself. Later a brief description of the organisation and structure of the code is given in order to ease the user interface at compile and link stage. Finally we will address how the library is actually built and illustrate its core features through the execution of proposed test drivers.

#### 2.1 THIRD-PARTY CODE

The library that we propose is composed by two so-called modules associated with a corresponding main function: the primary module, also referred to as the *focal* module, is the one used by the user to build executables and it implements all the essential methods that are required for the accomplishment of QUASIMONT's purpose, that is the computation of ad-hoc processed nodes and weights of the G-L quadrature formula in order to achieve double precise approximations of a definite integral with the minimum number of nodes possible. The *secondary* module provides supporting tools for the user to understand deeper the fundamental blocks of the monomial transformation s.a. the plot of the asymptotic estimate (1.8) and the computation of  $\beta_{\min}(n)$  and  $\beta_{\min}(n)$ . Although it is not essential for the correct functioning of the library, it features additional dependencies than the primary module and thus its compilation is kept separate from the rest of the code. In the following we address the building issues concerning the focal module and post-pone to Section 3.4 a brief description of the secondary module.

QUASIMONT relies on a number of third-party open-source libraries. Many of them usually come shipped with C++ itself e.g. the **standard** and **vector** libraries (required for basic data-structures and functions), the **algorithm** library (needed for sorting methods), the **math** library (used for basic mathematical operations s.a. fabs, pow and ceil) and others. There are however two more libraries, well-known in the scientific computing and open-source communities, that are linked to QUASIMONT (in the following the **v-number** indicates the minimum requirement to run our library):

- Boost C++ libraries (v-1.71) [1]: a vast, peer-reviewed, header-only collection whose primary tool in QUASIMONT is the Multiprecision library in which non-native higher precision f.p. formats have been implemented as C++ data-types. Of particular interest for our module is the IEEE 754 quadruple f.p. format which is supplied by Boost's library as a "GCC's \_\_float128 or Intel's \_Quad data types".
- GSL GNU Scientific Library (v-2.5) [6]: this rather well-known library is needed by QUASIMONT in only one occasion that is for the implementation of the integer degree polynomial solver gsl\_poly\_complex\_solve. In the library such method is used to extract the minimum number of quadrature nodes  $n_{\min}$  from the 7-th degree polynomial equation in (1.15). Alternative solvers and root-finders are available however in our case we were also interest in automatically locating the only real root of such polynomial (corresponding to  $n_{\min}$ , hence the choice we made.

Those dependencies need to be installed/compiled correctly on the user's machine; furthermore macros to each static library need to be included in the PATH environment variable in order to correctly link the objects files compiled from the source code. Luckily all the above libraries are easily downloaded and compiled in Linux using package managers, such as the **Advanced Package Tool** and the **Yellowdog Updater**, **Modified**, with a single command on the terminal. Moreover the aforementioned macros should be added automatically to the PATH variable.

```
Installation of third-party libraries

user@machine: home> # For Debian-like distros (Ubuntu, Mint, Knoppix, Kali ...)
user@machine: home> sudo apt-get update -y
user@machine: home> sudo apt-get install libboost-all-dev libgsl-dev
user@machine: home> # For RHEL-like distros (CentOS, Fedora, SUSE, Scientific Linux ...)
user@machine: home> sudo yum update -y
user@machine: home> sudo yum install install boost-devel gsl-devel
```

Additionally, QUASIMONT requires the proper installation of the appropriate building tools; at the present moment the library has been written for Linux platforms only and therefore we prioritized a minimalist and straightforward build process over cross-platform compliance by adopting the usage of makefile's (see Section 2.3). In it the default compiler specified for compiling and linking QUASIMONT's applications is GCC - GNU Compiler Collection [4]. The actual program that thus invokes the compilation of the library is GNU Make [5] which also requires to be correctly installed configured on the user machine. Also in this case the aforementioned package managers allow fast and simple installation of the tools with minimal input on the terminal.

```
Installation of building tools

user@machine: home> # For Debian-like distros (Ubuntu, Mint, Knoppix, Kali ...)
user@machine: home> sudo apt-get install build-essential
user@machine: home> gcc --version
user@machine: home> make --version
user@machine: home> # For RHEL-like distros (CentOS, Fedora, SUSE, Scientific Linux ...)
user@machine: home> sudo yum group install "Development Tools"
user@machine: home> gcc --version
user@machine: home> make --version
```

We remark that QUASIMONT's build has been achieved using versions 9.3.0 and 4.2.1 of GCC and GNU Make respectively. Once all the above packages and tools have been installed, the user should thoroughly check their correct configuration and if indeed links to their static libraries have been added to the PATH environment variable. The dependencies are large libraries although QUASIMONT uses a limited amount of the methods they provide; we therefore made sure that only the necessary parts of those were included in the source code, striving to maintain a clean and light final product. For the sake of completeness we hereby list all the methods implemented in those third-party libraries and that are used by QUASIMONT; those can be located in its source code, specifically in the leader file Quasimont.h, reported in the snippet below. As for any other source file in the library, a comment block precedes the code content, of which the first line specifies the location in the relative tree of the library (see Figure 2.1). It can be easily seen that all external source code headers are included in this single header file that takes the name of the library itself; following the definition of the aforementioned custom type it also includes the local headers of the library containing the declarations of all the functions implemented (see Section 2.2).

```
Quasimont.h
2 // File:
                 include/Quasimont.h
3 //
                 {\tt QUASIMONT-QUAdrature\ of\ SIngular\ polynomials\ using\ MONomial\ Transformations:}
4 // Library:
                            a C++ library for high precision integration of singular
                            polynomials of non-integer degree
6 //
7 //
8 // Authors:
                 Guido Lombardi, Davide Papapicco
9 //
10 // Institute: Politecnico di Torino
11 //
                 C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
                 Department of Electronics and Telecommunications (DET)
12 //
13 //
                 Electromagnetic modelling and applications Research Group
16 #ifndef QUASIMONT_H
17 #define QUASIMONT_H
19 #include <iostream>
20 #include <algorithm>
21 #include <iomanip>
22 #include <string>
23 #include <vector>
24 #include <tuple>
25 #include <fstream>
26 #include <stdlib.h>
27 #include <stdio.h>
28 #include <math.h>
29 #include <boost/math/constants/constants.hpp>
30 #include <boost/multiprecision/float128.hpp>
31 #include <gsl/gsl_poly.h>
33 namespace boomp = boost::multiprecision;
34 typedef boomp::float128 float128; // quadruple precision f.p. format
^{36} #include "Utils.h" // includes header file for plotting and other utilities ^{37} #include "DatIo.h" // includes header file for data I/O functions
38 #include "MonMap.h" // includes header file for functions computing the monomial map
40 #define EPS std::numeric_limits < double >::epsilon() // sets double machine-epsilon as

    → treshold

41 #define PI boost::math::constants::pi<float128>() // defines pi with 34 decimal digits
42 #define E boost::math::constants::e<float128>() // defines e with 34 decimal digits
44 template < typename type >
45 void quasimont(std::vector<type>& muntz_sequence, std::vector<type>& coeff_sequence);
47 #endif // QUASIMONT_H
```

Further down we find definitions of some constants used throughout the library and finally the declaration of leading access point of the primary module of the library, the method quasimont in which all other aforementioned methods of QUASIMONT converge and interact. This method is the focal point for all the aforementioned functions and acts as a sort of main-like function that is instead associate to the application itself (see Section 2.3). The definition of such method is given in the homonym source file Quasimont.cpp reported below. With emphasis on the focal module we refer to the latter source file as the focal method (or alternatively the access point from which each application of the library is built). On such file we highlight the comment block at the beginning of the definition of the function itself (lines 18-30) where the user finds quick useful insights about its usage, I/O and implementation. Such pattern is shared by each method across the main module of the library (see Chapter 4).

```
Quasimont.cpp
1 //---
2 // File:
               src/Quasimont.cpp
3 //
4 // Library:
               {\tt QUASIMONT-QUAdrature\ of\ SIngular\ polynomials\ using\ MONomial\ Transformations:}
                        a C++ library for high precision integration of singular
5 //
6 //
                        polynomials of non-integer degree
7 //
               Guido Lombardi, Davide Papapicco
8 // Authors:
9 //
10 // Institute: Politecnico di Torino
11 //
               C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
               Department of Electronics and Telecommunications (DET)
12 //
13 //
               Electromagnetic modelling and applications Research Group
14 //-
15
16 #include "Quasimont.h"
19 //
20 //
          FUNCTION: quasimont(muntz_sequence, coeff_sequence)
21 //
22 //
           INPUT: - muntz_sequence = sequence of real exponents of the polynomial
23 //
                  - coeff_sequence = sequence of real coefficients of the polynomial
24 //
          OUTPUT: - no outputs
25 //
26 //
27 //
       DESCRIPTION: access point of the focal module of the library where all the
28 //
                    primary methods are instantiated according to the user's input
29 //
31
32 template < typename type >
33 void quasimont(std::vector<type>& muntz_sequence, std::vector<type>& coeff_sequence)
34 {
   // PRINT INITIAL MESSAGE AND SELECTS USER INPUTS
35
   auto input_data = manageData(muntz_sequence, coeff_sequence);
36
37
   // EXTRACT N_MIN, BETA_MIN AND BETA_MAX
38
   auto monomial_data = streamMonMapData(std::get<0>(input_data));
39
40
   // COMPUTE THE MONOMIAL TRANSFORMATION ORDER
41
   double transf_order = computeMapOrder(std::get<1>(input_data), std::get<1>(monomial_data)
     \hookrightarrow );
43
   // COMPUTE AND EXPORT THE NEW G-L NODES & WEIGHTS
44
   auto quad_data = computeParamsGl(transf_order, std::get<0>(monomial_data));
45
46
   // CONVERTS AND EXPORTS NEW NODES AND WEIGHTS IN THE MOST OPTIMISED FLOATING-POINT FORMAT
47
     → POSSIBLE
48
   optimiseData(quad_data, muntz_sequence, coeff_sequence);
49 }
50 template void quasimont(std::vector<float128>& muntz_sequence, std::vector<float128>&
     51 template void quasimont(std::vector < double > & muntz_sequence, std::vector < double > &
```

#### 2.2 STRUCTURE

The source-code in the library does not use relative paths for finding the definitions of its methods in the headers; relative paths are instead used at compile and link time by the makefile (see Section 2.3). The user is nonetheless discouraged from moving files and/or changing those paths because they do appear occasionally in the source code for retrieving data from specific non-source files.

It is important therefore to understand where these files are stored and how the code is organised. As mentioned

in the previous chapters, QUASIMONT is not object-oriented and all its methods interact through the focal method quasimont that interfaces the user through the inputs defined in the main function. Aprt from it, all the remaining source code that constitutes the primary module of our proposed software is made of only 12 methods whose definitions are collected in one of the following three source files:

• MonMap.cpp contains every method associated with the computation of the monomial quadrature rule, ranging from the monomial map itself (i.e.  $\beta_{\min/\max}$ , r, etc...) to the quadrature parameters (i.e.  $\tilde{x}_j$ ,  $\tilde{w}_j$ ,  $J_{[a,b]}$ , etc...). To provide an easier reference for code debugging and amendment, a naming scheme of these methods is adopted; every function in this file is in fact named **compute**<**NameOfFunction**> as it can be evinced from the corresponding header file containing such functions' declarations

```
MonMap.h
2 // File:
                 include/MonMap.h
3 //
4 // Library:
                 QUASIMONT-QUAdrature of SIngular polynomials using MONomial Transformations:
5 //
                           a C++ library for high precision integration of singular
6 //
                           polynomials of non-integer degree
7 //
8 // Authors:
                Guido Lombardi, Davide Papapicco
9 //
10 // Institute: Politecnico di Torino
                C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
11 //
12 //
                Department of Electronics and Telecommunications (DET)
13 //
                Electromagnetic modelling and applications Research Group
14 //-
16 #ifndef MONMAP_H
17 #define MONMAP_H
19 // (SEE LINES 79~93 IN 'src/MonMap.cpp') Computes the optimal lambda_max when the input
      \hookrightarrow polynomial is a monomial and a maximum number of nodes is required
20 float128 computeLambdaMax(float128& lambda_min, int num_nodes);
21
_{22} // (SEE LINES 114^{\sim}129 IN 'src/MonMap.cpp') Computes the number of minimum quadrature nodes
      \hookrightarrow by finding the real root of the 7-th degree polynomial equation in (62)
23 int computeNumNodes(const float128& lambda_min, const float128& lambda_max);
24
    (SEE LINES 182~194 IN 'src/MonMap.cpp') Computes the order (r) of the monomial map as a
25 //
      \hookrightarrow linear interpolation of r_min and r_max
26 double computeMapOrder(const std::vector<float128>& lambdas, const std::vector<float128>&
      → betas);
27
28 // (SEE LINES 218~234 IN 'src/MonMap.cpp') Computes the new nodes and weights of the G-L

→ formula

29 std::tuple<std::vector<float128>, std::vector<float128>, std::vector

→ <float128>> computeParamsGl(const double& r, const int& n_min);

30
31 // (SEE LINES 349~365 IN 'src/MonMap.cpp') Computes the numerical integral with G-L
      \hookrightarrow quadrature formula
32 template < typename type1, typename type2 >
33 float128 computeQuadG1(const std::vector<type1>& nodes, const std::vector<type1>& weights,
      std::vector<type2>& muntz_sequence, std::vector<type2>& coeff_sequence);
35 // (SEE LINES 450~462 IN 'src/MonMap.cpp') Computes the a-posteriori relative error of the
      \hookrightarrow G-L quadrature using the new nodes and weights
36 template < typename type >
37 float128 computeExactError(const float128& In, std::vector<type>& muntz_sequence, std::
      → vector < type > & coeff_sequence);
39 #endif // MONMAP_H
```

• DatIo.cpp is the source file defining each method that does not perform raw computations but instead manages the data flow e.g. in I/O operations. Every function follows the naming scheme <NameOfFunction>Data emphasizing its characteristics of data manipulation method. The methods are declared in the corresponding header file

```
DatIo.h
2 // File:
                 include/DatIo.h
3 //
                 QUASIMONT-QUAdrature of SIngular polynomials using MONomial Transformations:
4 //
     Library:
                           a C++ library for high precision integration of singular
5 //
6 //
                            polynomials of non-integer degree
7 //
8 //
                 Guido Lombardi, Davide Papapicco
    Authors:
9 //
10 //
     Institute: Politecnico di Torino
                 C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
11 //
12 //
                 Department of Electronics and Telecommunications (DET)
13 //
                 Electromagnetic modelling and applications Research Group
14 //
16 #ifndef DATIO H
17 #define DATIO_H
18
19 // (SEE LINES 109~128 IN 'src/DatIo.cpp') Takes user-defined inputs from file
  template < typename type >
21 std::tuple<int, std::vector<float128>> manageData(std::vector<type>& muntz_sequence, std::
      → vector<type>& coeff_sequence);
  // (SEE LINES 258~271 IN 'src/DatIo.cpp') Extract the values of beta_min and beta_max
23
      \ \hookrightarrow \ \text{according} to the computed minimum number of nodes
24 std::tuple<int, std::vector<float128>> streamMonMapData(const int& comp_num_nodes);
25
    (SEE LINES 335 IN 'src/DatIo.cpp') Degrade the precision of the new G-L nodes and

ightarrow weights to establish minimum data-type for double precision quadrature
27 template < typename type >
  void optimiseData(std::tuple<std::vector<float128>, std::vector<float128>, std::vector<</pre>
      → float128>, std::vector<float128>>& quad_params, std::vector<type>& muntz_sequence,
      → std::vector<type>& coeff_sequence);
  // (SEE LINES 335~349 IN 'src/DatIo.cpp') Computes and exports the resulting G-L weights
30
      \hookrightarrow and nodes aling with other ouputs
31 template < typename type >
32 void exportNewData(const std::vector<type>& nodes, const std::vector<type>& weights, const

    std::vector<float128>& output_data);

33
34 #endif // DATIO_H
```

• VecOps.cpp finally defines every function that does not either perform direct computations for the quadrature rule nor it performs I/O operations on data; instead the methods instantiated from the source file are used to automatise specific operations on vectors that are required multiple times across the library specifically casting vectors' values in higher-than-double floating-point format (implemented in method in castVector) and the doubleDotProduct which implements a precise inner product operation between two non-scalar vectors with high precision avoiding numerical cancellations of smaller-than-epsilon values. Given the generic nature of their task, no naming scheme is assigned to these methods whose declarations are found in the header file Utils.h below. In the latter we also find declarations of the 3 methods of the secondary module that are all defined, alongside its main, in the ErrTools.cpp source file (see Section 3.4).

```
Utils.h
                 include/Utils.h
3 //
4 // Library:
                 QUASIMONT-QUAdrature of SIngular polynomials using MONomial Transformations:
                           a C++ library for high precision integration of singular
5 //
6 //
                           polynomials of non-integer degree
7 //
8 // Authors:
                Guido Lombardi, Davide Papapicco
9 //
10 // Institute: Politecnico di Torino
                C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
11 //
12 //
                Department of Electronics and Telecommunications (DET)
13 //
                Electromagnetic modelling and applications Research Group
14 //-
16 #ifndef UTILS H
17 #define UTILS_H
19 // (SEE LINES 22~31 IN 'utilities/VecOps.cpp') Returns the float128 input vector in a type
      \hookrightarrow specified by the instatiantiation
20 template < typename type >
21 std::vector<type> castVector(const std::vector<float128>& input_vector, const type&

    type_infer);
22
_{23} // (SEE LINES 22\ ^{\circ}31 IN 'utilities/VecOps.cpp') Computes the inner product between two
      \hookrightarrow vectors (of the same type) avoiding numerical cancellation
24 template < typename type >
25 float128 doubleDotProduct(const std::vector<float128 & f_values, const std::vector<type>&
      → weights);
26
27 // (SEE LINES 22~31 IN 'utilities/VecOps.cpp') Generates n equispaced points between two
      \hookrightarrow input real numbers
28 template < typename type >
29 std::vector<type> linspacedVector(const type& start_type, const type& end_type, const int&
      → num_steps);
30
31 // (SEE LINES 22~41 IN 'utilities/ErrTools.cpp')
32 template < typename type >
33 type aPrioriAsympEstimate(const type& input_lambda, const int& num_nodes);
35 // (SEE LINES 22~41 IN 'utilities/ErrTools.cpp')
36 template < typename type >
37 void plot(const int& num_nodes, const type& beta_min, const type& beta_max);
39 // (SEE LINES 22~41 IN 'utilities/ErrTools.cpp')
40 void printProgressBar(const int& iter, const int& num_iter);
42 #endif // UTILS_H
```

Now that we have a clearer idea of the actual content of QUASIMONT source code let us discuss, with visual reference depicted in Figure 2.1, the organisation of each file in the library's directory. Source files of the primary module, i.e. MonMap.cpp and DatIo.cpp are located in the subdirectory QUASIMONT/src alongside Quasimont.cpp itself. On the other hand VecOps.cpp is placed in the QUASIMONT/utilities subdirectory where we can also find the secondary module source code ErrTools.cpp. Despite such separation, all the header files outlined above (one per source file of the focal module) are located in the QUASIMONT/include subdirectory, including Quasimont.h. Now we discuss the aforementioned relative paths; we mentioned that they are essentials for the correct loading of raw data from tabulated data-files into the source code.

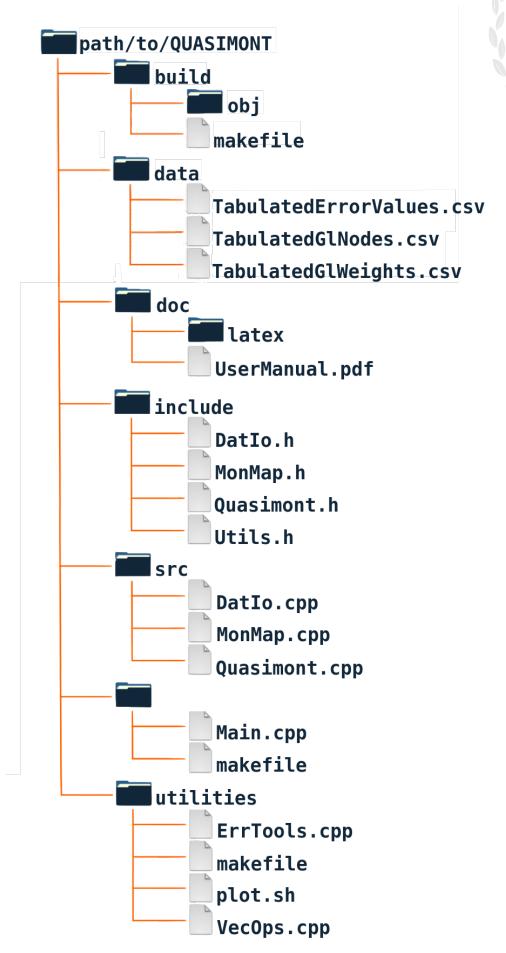


Figure 2.1: A directory tree representing the structure and organisation of QUASIMONT



Those files are:

- TabulatedErrorValues.csv collecting the values of  $\beta_{\min}(n)$  and  $\beta_{\max}(n)$  for each even value of  $n \in [10, 100]$ ;
- TabulatedGlNodes.csv storing the G-L quadrature nodes in [-1,1] for each even value of  $n \in [10,100]$ ;
- TabulatedGlWeights.csv storing the strictly positives, symmetric (w.r.t. to 0) weights of the G-L quadrature formula for each even value of  $n \in [10, 100]$ .

Those files are located in **QUASIMONT/data** and shall never be changed. In the **QUASIMONT/build** the makefile used for building the library and its applications is located whereas **QUASIMONT/build/obj** subdirectory contains the object files created at compile-time. Finally, test drivers (see Section 2.4) used for checking the proper installation and execution of the application are located in **QUASIMONT/test**.

#### 2.3 BUILD PROCESS

The principle by which QUASIMONT is used is that of creating executables, henceforth referred to as **applications**, through the compilation and linking of the library's source code and a Main.cpp file containing the user's input thus called **input source file** (see Section 3.1). We define a one-to-one correspondence between any specific main of the primary module and its associated application.

```
Application's own (top-level) makefile
  # File:
               build/makefile
4 #
    Library:
               QUASIMONT-QUAdrature of SIngular polynomials using MONomial Transformations:
                          a C++ library for high precision integration of singular
5
                          polynomials of non-integer degree
6 #
7 #
8 #
   Authors:
               Guido Lombardi, PhD, Davide Papapicco
10 # Institute: Politecnico di Torino
11 #
               C.so Duca degli Abruzzi, 24 - Torino (TO), Italia
               Department of Electronics and Telecommunications (DET)
12 #
               Electromagnetic modelling and applications Research Group
 #
14
15
16 CXX = g++
17
18 INCDIR = ../include
19 SRCDIR = ../src
20 UTLDIR = ../utilities
21 OBJDIR = obj
22
23 UTL = $(UTLDIR)/VecOps.o
24 OBJ = $(OBJDIR)/Quasimont.o $(OBJDIR)/DatIo.o $(OBJDIR)/MonMap.o
26 CXXOPTIONS = -g -ansi -std=c++17
  CXXFLAGS = $(CXXOPTIONS) -I $(INCDIR)
27
28
 dafault: $(OBJ)
30
31 $(OBJDIR)/%.o: $(SRCDIR)/%.cpp $(INCDIR)/*.h
    $(CXX) -c $< -o $0 $(CXXFLAGS)
32
33
34 $(OBJDIR)/VecOps.o: $(UTLDIR)/VecOps.cpp $(INCDIR)/Utils.h
    cd $(UTLDIR) && $(MAKE)
35
36
37 static: $(OBJ) $(OBJDIR)/VecOps.o
    ar rcs libquasimont.a $^
38
39
40 clean:
    rm -f $(OBJDIR)/*.o
41
```

The build process is based on the recursive make approach, i.e. the input source file is built through a top-level makefile that recursively invokes the makefile responsible for building the source code of the library, its utilities and third-party dependencies. The library source code shall be compiled just once and be available thereafter for linking each new application unless the rule allclean is invoked (which deletes the library's object files). This practice is useful for users of the library that only require to execute standalone applications and can thus reuse the compiled objects of the source code multiple times with no changes. On the other hand, if integration of QUASIMONT in larger, more complex code is required (e.g. in FEM/BEM libraries), linking to the static library is necessary. It is later explained in Section 2.4 that QUASIMONT is shipped with a reference application in QUASIMONT/test which, among other things, exemplifies the build sequence of the library.

```
Compilation and Linking of the library
# First clean the object files from any previous compilation ...
   ../build && make clean
make[1]: Entering directory '/home/QUASIMONT/build'
make[1]: Leaving directory '/home/QUASIMONT/build'
# ... then builds the library object files
cd ../build && make
    -c ../src/DatIo.cpp -o obj/DatIo.o -g -ansi -std=c++17 -I ../include
      ../src/MonMap.cpp -o obj/MonMap.o -g -ansi -std=c++17 -I ../include
make[1]: Leaving directory '/home/QUASIMONT/build'
cd ../utilities && make ../build/obj/VecOps.o
make[1]: Entering directory '/home/QUASIMONT/utilities'
g++ -c VecOps.cpp -o ../build/obj/VecOps.o -g -ansi -std=c++17 -I ../include
make[1]: Leaving directory '/home/QUASIMONT/utilities
# ... and finally links all together to create the executable ...
   ../build/obj/*.o -o Test -lm -lquadmath -lgsl -lgslcblas
# ... which is then ran!
./Test
               ** QUASIMONT **
 Input polynomial...
```

The output of the compilation of the source files are object files that will be stored in the QUASIMONT/build/obj subdirectory as explained previously. The linking of those objects is invoked only by the top-level makefile associated to the specific application. For each application built by the user it is considered a good practice to invoke the clean rule prior to the build process itself, as shown above. We emphasize that, with the exception of those cases when QUASIMONT is used as a tool in a larger library, each application should be associated to its own subdirectory located within QUASIMONT itself. In this subdirectory a user input source file containing the main, named Main.cpp by default, should be located. User can name it whatever it wants as long as it is consistent with the one reported in the top-level makefile of the application, which should also be located in the subdirectory. Nonetheless we suggest to retain the naming convention reported in the makefile above, that is the application (Test in our example above) should be name according to the directory in which is located (i.e. test) whereas the input source file should be always named Main.cpp to provide easier reference for debugging.

#### 2.4 INSTALLATION AND TEST DRIVER

Installation of the library can be done by building the Main.cpp input source file in the QUASIMONT/test subdirectory, which contains the test driver benchmarking QUASIMONT's performance. The Test application built from it runs the library's processing methods onto three generalised and classical polynomial integrands that introduce the user to the library interaction, execution and output whilst assuring that the core functionalities have been compiled correctly (no conflict at linking stage occurs). The three polynomial functions are the following

$$p_1(x) = 5x^{-\frac{\pi}{4}} - x^{-\frac{1}{2}} + 1 + 10x^2 + ex^{e+\frac{1}{4}}$$

$$p_2(x) = x^{-\frac{e}{3}}$$

$$p_3(x) = x^{17} + x^{35}$$

and, with the exception of  $p_3(x)$ , all have a singularity in [0,1], which is also the integration interval set by default in QUASIMONT. Once both the library's and user input's source files have been compiled and linked into the corresponding executable, the resulting application integrates each polynomial using the monomial quadrature rule; a list of important information regarding both the I/O and the monomial transformation itself is displayed on the terminal whereas the main results, which we emphasize to be the new processed G-L quadrature nodes and weights, are exported in the associated subdirectory (see Section 3.2). The user should check its content and verify that the data contained in it matches what is reported in the following tables 2.1, 2.2, 2.3 for the specific polynomial functions. Once satisfied the user can then return to the CLI where the program is waiting for her/him to go ahead to the next benchmark.

```
Building and executing the test driver:
                                                              p_1(x)
user@machine: home/QUASIMONT/test> make clean
   -r output
user@machine: home/QUASIMONT/test> make
g++ -c Main.cpp -o ../build/obj/Main.o -g -I ../include
    ../build && make
make[1]: Entering directory '/home/QUASIMONT/build'
g++ -c ../src/Quasimont.cpp -o obj/Quasimont.o -g -I ../include
g++ -c ../src/DatIo.cpp -o obj/DatIo.o -g -I ../include
g++ -c ../src/MonMap.cpp -o obj/MonMap.o -g -I ../include
make[1]: Leaving directory '/home/QUASIMONT/build'
make[1]: Entering directory '/home/QUASIMONT/utilities'
g++ -c Utils.cpp -o ../build/obj/Utils.o -g -I ../include
make[1]: Leaving directory '/home/QUASIMONT/utilities'
g++ ../build/obj/*.o -o Test -lm -lgsl -lgslcblas -lgmp -lquadmath
./Test
         ** MONOMIAL QUADRATURE RULE **
 Input polynomial p(x) = +2.71828*x^{(2.96828)}+5*x^{(-0.785398)}-1*x^{(-0.5)}+x^{(0)}+10*x^{(2)}
    Accepted sequence of exponents **
    Lambda_min = -0.785398, Lambda_max = 2.96828 **
    Beta_min = 4.37782518, Beta_max = 127.894326 **
 ** I_n(p(x)) = 26.3172973764883195713082386646419764 **
     E_n(p(x)) = 1.34995384517502488806263407884576529e-16 **
PROGRAM TERMINATED! Results are available in the 'output' subdirectory.
```

The correct execution of all three benchmarks will then close the application. The user should check that each benchmark is executed without problems and the results are correctly generated (see Section 3.2). As for the the quality of the results obtained for those tests, an in-depth analysis, coupled with the fast execution of the program, shows the advantages provided by QUASIMONT over classical G-L and other generalised quadrature rules. The first polynomial  $p_1(x)$  is a model proposed at equation (73) in [8], Section 5.1. Example 1 and it represents the quintessential integrand function, often encountered in the numerical methods for differential and integral equations, on which QUASIMONT is deemed necessary. The generalised polynomial feature a strong singulairty in the infimum of the interval and all but one of its monomial terms have non-integer degree. The numerical approximation of the integral is achieved with n = 32 nodes using a monomial transformation of high order of the classical G-L nodes and weights in [0,1].

Transf	formed G-L nodes and w	veights (double f.p. format)
$j \in \mathbb{N}$	$x_j \in [0,1]$	$w_j \in \mathbb{R}^+$
0	4.0256721894941735e-83	2.9709584266857193e-81
1	2.2116841854653406e-62	7.1971053989801097e-61
2	3.4370358897566318e-51	7.1255611223692978e-50
3	1.6010758830624544e-43	2.4253789034229506e-42
4	1.0479208102676717e-37	1.2456363438765983e-36
5	4.8718071131884711e-33	4.7453741025535338e-32
6	3.7119919463646725e-29	3.0494845207591382e-28
7	7.5510919371932376e-26	5.3393428605147779e-25
8	5.58947068987428e-23	3.4526789629984772e-22
9	1.8549840400142102e-20	1.0121884313459638e-19
10	3.1981531227726135e-18	1.5545919457374846e-17
11	3.1905126409913618e-16	1.3904418738462426e-15
12	1.9974633805093215e-14	7.8421013950383668e-14
13	8.3548669580378659e-13	2.9653252968844048e-12
14	2.4525558094710645e-11	7.8879379262599627e-11
15	5.2553535644885825e-10	1.5337625816699302e-09
16	8.4865615532959245e-09	2.2485149221054993e-08
17	1.0601166175497224e-07	2.5487504629916981e-07
18	1.0467771915132323e-06	2.2805293469267595 e-06
19	8.3187859060800558e-06	1.6383778757563812e-05
20	5.4017656350748472e-05	9.583886949817516e-05
21	0.00029027719974030597	0.00046172220499588948
22	0.0013048618829373392	0.0018488842315729846
23	0.0049515587664587246	0.0061972140073356637
24	0.01598386920155067	0.017474549464975012
25	0.044176504650425052	0.041563995305652503
26	0.10510275956828145	0.083385319613667491
27	0.21621415218381346	0.14051580648196024
28	0.38598199665949656	0.19670495174814193
29	0.59964365548997856	0.22295968412650397
30	0.81242716007987004	0.1915755472071223
31	0.96137880664253184	0.097197543454586643

Table 2.1: New G-L nodes and weights obtained by a monomial transformation of order r = 28.77 integrating  $p_1(x)$  in [0,1].

From the table above it is easy to get a sense on what was displayed in the previous Figure 1.2; the classical nodes G-L nodes of the associated quadrature rule with n=32 are in fact distributed symmetrically in [0,1] with an equal abundance of those at both bounds of the integration interval. Conversely here, the monomial transformation order shifts those nodes consistently towards the lower bound a=0, squashing the vast majority of them (26 out of the total 32) inside the sub-interval [0,0.1] where the singularity is captured. Onto the second polynomial, it is proposed with the purpose of introducing the user to a core functionality of QUASIMONT that requires further input on the CLI. We see in fact that  $p_2(x)$  is a monomial of non-integer degree and, as stated in Section 1.1, their numerical integration requires careful manipulation. During the modelling process of larger applications, especially when dealing with finite elements constructed over triangulations of domains with singular spatial geometries, there

may in fact arise the need of integrating low order, singular and hyper-singular polynomial basis functions. One straightforward workaround, which is in actuality often encountered in many of those problems, is the addition of a higher-order monomial function. In QUASIMONT we allow for the insertion of such term by identifying its degree as  $\lambda_{\text{max}}$ ; the additional monomial will have a unitary coefficient by default and can indeed be the constant  $x^0 = +1$  itself. The integration is enabled using a caveat prompted on the terminal and it consists in choosing one path between two mutually exclusive options that the user must exercise in order to continue with the application. One of those is the choice of specifying the maximum number n of nodes it wants for the quadrature rule, in which case the library will automatically compute  $\lambda_{\text{max}}$  and thus integrate  $\tilde{p_2}(x) = x^{-\frac{e}{3}} + x^{\lambda_{\text{max}}}$ . The second path allows instead to specify  $\lambda_{\text{max}}$  directly and let QUASIMONT carry out the integration.

It is easy to see that the second case essentially reduces to a "standard" polynomial input, as far as the library is concerned. Therefore we suggest the user to go ahead with the former option and specify the maximum n for which its singular monomial can be integrated. The user should therefore type nodes on the CLI and press Enter; we are now prompted to select any value of  $n \in [10, 100]$ ; user should type 12 and press Enter again. On the contrary typing lambda will cause the application to resort to its original workflow with the intermediate step of requiring the input of the value of  $\lambda_{\text{max}}$  with the ... character separating the integer from the decimal entries.

```
Building and executing the test driver: p_2(x)

How do you want to proceed?

[enter 'nodes' to specify the number of nodes or 'lambda' for the exponent]

Input: nodes

Please specify the desired number of quadrature nodes (number must be even): 12

**** Beta_min = 8.54130275, Beta_max = 23.2002133 **

** Accepted sequence of exponents **

{-0.906093942819681745120095823784220804, -0.761820098074495688500462620140751824}

** Lambda_min = -0.906093942818681745120095823784220804, Lambda_max =

→ -0.761820098074495688500462620140751824 **

*** Beta_min = 8.54130275, Beta_max = 23.2002133 **

** Transformation order = 101.604763 **

*** Using float50 format for nodes and weights

** I_n(p(x)) = 14.8474473958169998935662658402046966 **

** E_n(p(x)) = 3.024552613045830084165988346191664263e-16 **

PROGRAM TERMINATED! Results are available in the 'output' subdirectory.

Press any Key to exit
```

We make the remark that any miss-typed or empty input, will cause QUASIMONT to throw an error message and exit the program. As we can see QUASIMONT computes automatically a value of  $\lambda_{\rm max} = -0.761820098074$  and the resulting quadrature retains the machine-epsilon double precision. Here The library is stressed more as its transformation order gains an order of magnitude; the effects are registered on the mapped nodes and weights listed in the following table.

Transf	Transformed G-L nodes and weights (double f.p. format)			
$j \in \mathbb{N}$	$x_j \in [0,1]$	$w_j \in \mathbb{R}^+$		
0	1.6049071040670031e-207	4.1718913867161883e-205		
1 1	8.9928778579205101e-135	1.0190834572864527e-132		
2	3.8114927390083667e-96	2.6942018712200615e-94		
3	2.2836535914412963e-70	1.1423068956574762e-68		
4	1.5051778942712652e-51	5.6486159643104545e-50		
5	3.2351037993447086e-37	9.3619397179684863e-36		
6	4.1726571491647704e-26	9.3872826135408085e-25		
7	1.7198033365919789e-17	2.9828626539946124 e-16		
8	6.3435088215964896e-11	8.2496166241381113e-10		
9	4.0434975152747609e-06	3.7158177341626430e-05		
10	0.0067940636342241	0.0387692527955493		
11	0.3901949656940479	0.9438508439664283		

Table 2.2: New G-L nodes and weights obtained by a monomial transformation of order r = 101.6 integrating  $p_2(x)$  in [0,1].

The reason for such an extreme value of the map is that we specified the maximum number of quadrature nodes to be used is n=12; such value force the algorithm to compress the region of finite-arithmetic exactness to a very narrow sub-interval of  $\lambda \in (-1, +\infty)$  and hence the extreme pinching of the G-L nodes on the lower bound a=0. Finally, with the last benchmark a classical polynomial of high integer-degree is integrated following the processing of the G-L nodes and weights. As  $p_3(x)$  is a binomial, the standard path of QUASIMONT is ran. According to the properties described in Section 1.2.2, it would only require  $n=\frac{d+1}{2}=18$  nodes for the classical G-L quadrature to achieve double precise integration.

Yet we immediately notice that QUASIMONT outperforms such result using even less samples in [0,1], i.e. n=12; also the transformation order needed by the monomial map is significantly lower than the previous two cases. The integer degrees of the integrand function thus makes the polynomial suitable to very little rearrangement of the classical nodes distribution and weights positive values in order to achieve a numerical approximation that is accurate within the machine-epsilon. This can be assessed by the table below by how close those processed values are, w.r.t. the classical G-L nodes in [0,1], when compared to those of the previous generalised cases of  $p_1(x)$  and  $p_2(x)$ .

Transf	Transformed G-L nodes and weights (double f.p. format)		
$j \in \mathbb{N}$	$x_j \in [0, 1]$	$w_j \in \mathbb{R}^+$	
0	0.0597707229696358	0.0919264663553836	
1	0.1610307309568925	0.1079664407846363	
2	0.2725515941208583	0.1139863183561349	
3	0.3872246099856674	0.1145999654489373	
4	0.5003873977306973	0.1111039615531504	
5	0.6082809536783961	0.1041479683059256	
6	0.7076854327640707	0.0941968566214454	
7	0.7958143666363263	0.0816648573999376	
8	0.8702918448156044	0.0669634924046180	
9	0.9291601555462656	0.0505192348221430	
10	0.9708981507831240	0.0327793590987762	
11	0.9944473508291223	0.0142322139984140	

Table 2.3: New G-L nodes and weights obtained by a monomial transformation of order r = 0.6011 integrating  $p_3(x)$  in [0,1].

With these results we would like to direct the user attention on the possibility of using QUASIMONT even for standard/classical polynomials of integer degree as its processed nodes and weights will most likely lead to a fewer samples in the quadrature rule and thus more efficient code in the numerical analysis of complicated physical models. At the best of our knowledge, and based on the tests reported here and in [8, 9], the monomial transformation can be adapted to the widest range of generalised polynomial of non-integer degree as long as the constraint of  $\lambda_{\min} > -1$  holds for the integrand. By excluding those cases of rational functions we argue that the usage of QUASIMONT produces accurate results faster (using the minimum possible number of samples) and more efficiently (outputting the most optimised f.p. formats for the G-L quadrature parameters) than any other algorithm that

currently deals with both classical and singular polynomial integrands of either integer and/or non-integer degree. As a final important observation, we note that QUASIMONT uses tabulated values of the original G-L nodes and weights in [-1,1] with 50 decimal digits of precision; the automatisation of those is outside the scope of the library and already explored in details and implemented in other works [3,7].



# USER INTERFACE

The execution of the test drivers should have introduced the user on the fundamentals and interaction with the library. It is now time to expose its I/O interface and enabling the user to the creation of a quick application. In the following chapter we shall provide a step-by-step procedure to setup, build and execute a custom-made application from scratch. In the first section we discuss the input source file, amendable by the user to create her/his first application with the library. In the second section we address how the results are exported. Finally we briefly address how these results can be used by other applications and loaded in external code automatically by integrating QUASIMONT in a larger library and conclude with a brief touch on the secondary module of our library.

#### 3.1 THE INPUT SOURCE FILE

Let us start with an example; we would like to integrate the following singular polynomial

$$p(x) = x^{\frac{\pi}{2}} + x^{\frac{\pi}{3}} + x + x^{\frac{\pi}{6}} + 1, \quad x \in [0, 1]$$

which is reported in Section 5.6. Example 6 in [8]. We start by creating a new source file collecting our inputs. By recalling Main.cpp in the QUASIMONT/test subdirectory we can create a copy of the whole subdirectory and rename it accordingly, e.g. QUASIMONT/MyApp

```
Creation of application's directory

user@machine: home/QUASIMONT> cp -r test MyApp
user@machine: home/QUASIMONT> cd MyApp/
user@machine: home/QUASIMONT> rm -r output/ Test
```

Now that a new application directory exists it is necessary to change our inputs in both the input source file and the associated top-level makefile. We start from the latter for which the amendments amount to

- at lines 33, 34 and 46 (see the code snippet in Section 2.3) change the string Test to MyApp to effectively rename the application built by the compiler;
- alternatively at line 31 define a macro variable EXE\_NAME = MyApp and invoke it as \$(EXE\_NAME) at the corresponding lines above.

With regards to the input source file we must Main.cpp in a text editor or IDE and observe the content of the test driver; going ahead and delete the comment block at lines 1-14 and all the code in the main will prepare it for

our next inputs. We remind that QUASIMONT is designed to perform its operations on generalised polynomials with strong endpoint singularities in [0,1] therefore, by using such bounds as the default integration interval, the library only requires the user to uniquely specify its input i.e.

- the coefficients\_sequence stored in a std::vector of length r+1=5 (see Sub-section 1.2.4);
- the muntz\_sequence of exponents of the polynomial p(x) (notice that the exponent of the constant term is 0 as in  $x^0 = +1$ ) also stored in a std::vector of the same length

If the two data-structures have different lengths, QUASIMONT will throw an error message and exit the program.

```
(input source file)
  Main.cpp
 #include "Quasimont.h"
     main(int argc, char** argv)
4
    std::vector<double> interval = {0, 1};
    std::vector<float128> coefficients_sequence = {1, 1, 1, 1, 1};
    std::vector<float128> muntz_sequence = {0,
                                             1.
                                             boost::math::constants::pi<float128>()/2,
                                             boost::math::constants::pi<float128>()/3,
10
                                             boost::math::constants::pi<float128>()/6};
12
    quasimont(muntz_sequence, coefficients_sequence, interval, plots);
13
14
    return 0;
15 }
```

Order of input of either muntz\_sequence and coefficients\_sequence does not matter as QUASIMONT automatically extract  $\lambda_{\min}$  and  $\lambda_{\max}$  through a sorting algorithm. Regardless of the "absolute" order, it is trivial that the user must make sure that the "relative" order of the two sequences must coincide. Once we correctly defined all the inputs we can instantiate the focal method quasimont, then save the amended file and exit the editor.

#### 3.2 RESULTS AND OUTPUTS

We can go ahead and build the application using the command make on the terminal. In the top-level makefile of the Test application we embedded the automatic execution of the program once the compilation is (successfully completed). Should the user deemed it necessary it can be disabled by erasing line 34 of the makefile and then manually input ./MyApp on the CLI at the end of the compilation. Ragardless, once the application is ran the first feedback to the user is its input followed by the computed parameters of the monomial map i.e.  $\lambda_{\min} \ \lambda_{\max} \ \beta_{\min} \ \beta_{\max} \ r$ . The next information is the floating-point format with which the new processed G-L nodes and weights have been exported (see below for further explanation) and lastly the value of the numerical integral and its remainder. The classical G-L parameters are stored in TabulatedGlNodes.csv and TabulatedGlWeights.csv in text format and imported in the source code as float 50 having themselves 50 digits of precision. Since doubleprecision quadrature can be achived with lower precision data, QUASIMONT features a method called degradeData (see Sub-section 4.2.5) that automatically selects the most optimised format possible, among those listed in Section 2.1, with which to export the output processed G-L parameters. The optimality here is meant as the lowest-precision f.p. format that still allows to retain a machine-epsilon accuracy (we have selected the double precision) for the relative error of the integral computed through the monomial quadrature rule. These results are not shown on the terminal but are instead exported in three separate files called Results.txt , Nodes.txt and Weights.txt , all located in the QUASIMONT/MyApp/output subdirectory created automatically by the application.

The former file collects input and outputs of the library alongside the values of the numerical integral approximated using both the classical and monomial G-L quadrature rule; this file is therefore intended for the user to have an immediate feedback on the quality of the approximation made by QUASIMONT. The remaining two files, as their name suggest, list the actual output of the library i.e. the new processed G-L nodes and weights respectively; the user should reference her/his results with those listed in the following Table 3.1

Transf	Transformed G-L nodes and weights (double f.p. format)			
$j \in \mathbb{N}$	$x_j \in [0,1]$	$w_j \in \mathbb{R}^+$		
0	2.496873777589448e-22	6.382643308743462e-21		
1	3.6337082916294261e-15	4.0633638229333794e-14		
2	2.4125934202252856e-11	1.6938542774252765e-10		
3	9.0001024671145157e-09	4.5171103120777135e-08		
4	7.1605972089111044e-07	2.7362368857409751e-06		
5	2.128638447833919e-05	6.4045740108986223e- $05$		
6	0.00031536400723379104	0.00075986216719157779		
7	0.0027510867463825276	0.0053358521063752865		
8	0.015684540279573143	0.024358682386555443		
9	0.062590590794555256	0.076515361899770665		
10	0.18315194992283396	0.17036173107876987		
11	0.40570033065293948	0.26937128724008813		
12	0.69503783727311896	0.28843004674283595		
13	0.93360229278243201	0.16480034906088914		

Table 3.1: New G-L nodes and weights obtained by a monomial transformation of order r = 9.98 integrating the generalised polynomial p(x) defined above for this custom application.

They are exported with the f.p. precision that has been automatically established by the aforementioned degradation and the user is assured to use those to achieve double machine-epsilon in terms of the quadrature remainder. For this reason we made the design decision not to carry the output of the library as a return data structure of the focal method quasimont but instead use the string native data-type and export them in text file as to preserve the optimised precision with which they have been calculated.

#### 3.3 STATIC-LIBRARY AND SOFTWARE INTEGRATION

So far we addressed those interactions with the library that are self-contained in the single application created by the user with QUASIMONT; our hope however is that our proposed routine is used in larger mathematical software in numerical analysis and scientific simulations. For this reason we decided to embed the possibility of creating a static library to which the user can easily link when building any other C++ software. This option enables the user to integrate with ease the focal module quasimont without few other adjuestments required to load its outputs.

First and foremost the static library libquasiment.a should be created in **QUASIMONT/build** by invoking the non-default rule make static of the makefile in the aforementioned subdirectory.

```
User@machine: home/QUASIMONT> cd build/
user@machine: home/QUASIMONT/build> make static
g++ -c ../src/Quasimont.cpp -o obj/Quasimont.o -g -ansi -std=c++17 -I ../include
g++ -c ../src/DatIo.cpp -o obj/DatIo.o -g -ansi -std=c++17 -I ../include
g++ -c ../src/MonMap.cpp -o obj/MonMap.o -g -ansi -std=c++17 -I ../include
g++ -c ../src/MonMap.cpp -o obj/MonMap.o -g -ansi -std=c++17 -I ../include
cd ../utilities && make
make[1]: Entering directory '/home/QUASIMONT/utilities'
g++ -c Utils.cpp -o ../build/obj/Utils.o -g -ansi -std=c++17 -I ../include
make[1]: Leaving directory '/home/QUASIMONT/utilities'
ar rcs libquasimont.a obj/Quasimont.o obj/DatIo.o obj/MonMap.o obj/Utils.o
```

The link to the static library is created, when building the external software, by the user by specifying the absolute or relative paths (at her/his own discretion) to:

- the QUASIMONT/include subdirectory containing the library header files, which is done by adding the flag

  -Ipath/to/QUASIMONT/include to the GCC compiler options;
- the actual lib quasimont.a itself by adding path/to/QUASIMONT/build/lib quasimont.a to the GCC linker option

Therefore, if the user wants to build an external App with QUASIMONT, those two GCC options must be appended during its own buildining process. If the App is built using the makefile then those commands are to be added to the appropriate rules, as reported in the example below

```
External software's makefile

default: App.o

g++ App.o -o App path/to/QUASIMONT/build/libquasimont.a -lm -lgsl -lgslcblas -lgmp -

output lquadmath

App.o: App.cpp

g++ -c App.cpp -o App.o -g -ansi -std=c++17 -Ipath/to/QUASIMONT/include
```

It is important to notice that the linking of the third-party dependencies previously outlined (see Section 2.1) is carried over the user's own software in order to integrate QUASIMONT correctly. Also, it should be made explicit the need for including the focal header file Quasimont.h in the software's App.cpp source code in order to avoid undefined references to QUASIMONT's methods. This is clearly exemplified in the snippet below showing the content of a minimalist App that simply instantiates the focal module quasimont of our library and then terminates. We make the final observation that, in order for the App to make use of QUASIMONT's main outputs it must load the new processed G-L nodes and weights in the external code from the text files that are generated by our library.

#### App.cpp (user's external source code) #include "Quasimont.h" 3 int main() 4 { std::vector <float128> coeff\_sequence = {1, 1, 1, 1, 1}; 5 std::vector <float128> muntz\_sequence = {0, boost::math:: constants ::pi<float128 >()/2, boost::math:: constants ::pi<float128 >()/3, 9 boost::math:: constants ::pi<float128 >() /6}; 10 11 quasimont(muntz\_sequence, coeff\_sequence); 12 13 // Da inserire qui il loading dei pesi e nodi trasformati da quasimont attraverso // i files output/Nodes.txt e Weights.txt 15 16 17 return 0; 18 }

Now the user will be able to use QUASIMONT in her/his external software/source code and exploit its results for the her/his own needs. As a final remark we note that, because of the relative paths to the raw data (see Section 2.2), the folder QUASIMONT/data must necessarily be copied one level above the the software's App.cpp source code that instantiates quasimont from the static library. If such subdirectory is not placed properly the library will fail to locate the necessary .csv files needed for its execution and subsequently throw an run-time error.

#### 3.4 ADDITIONAL SUPPORTING AND VISUAL TOOLS

To conclude the user interface with our library we will illustrate the additional functionalities that we embedded in QUASIMONT's secondary module. As superficially mentioned in Section 2.2, all the content of the secondary module is provided by the unique ErrTools.cpp source file. In it, aside for the main function, we implemented four methods instantiated in the main. They are particularly simple and as such do not need a detailed explanation aside for the fact that they all concur to generate:

- the exact same tabulated data TabulatedErrorValues.csv of  $\beta_{\min}(n)$  and  $\beta_{\max}(n)$  that is available in QUASIMONT/data;
- the plot of the novel asymptotic error estimate (1.8) for a given, user-specified, value of n.

The user can compile and execute the secondary module by invoking the rule tools for the application's top level makefile. The results will be stored in the run-time created **QUASIMONT/utilities/estimate** subdirectory. If the users re-compiles the source code of the secondary-module by specifying a different value for n, the previously obtained plots and error values will not be over-written.

```
Compilation and execution of QUASIMONT's secondary module

user@machine: home/QUASIMONT/test> make tools
cd ../utilities && make tools
make[1]: Entering directory '/home/QUASIMONT/utilities'
g++ -o Tools ErrTools.cpp -lmpfr -I ../include
./Tools

Computing for n = 10
    beta_min = 13.5722147
    beta_max = 14.0059
Computing for n = 12
    beta_min = 8.5...
```

The secondary module has two additional dependencies w.r.t. the focal module, which is part of the reason why we decide it to keep them separated in their implementation. Those are

- GNU MPFR [2]: based on GMP GNU Multi Precision library, and interfaced with QUASIMONT via Boost Multiprecision library's back-end wrapper classes, it provides access to *higher-than-quadruple* f.p. formats which are necessary for the evaluation of the Euler's Gamma function in the computation of the asymptotic error estimate (1.8).
- Gnuplot: the world-famous, cross-platform utility used for plotting scientific charts and used by the shell script plot.sh in the QUASIMONT/utilities subdirectory.

As for the focal module, those need to be installed correctly on the user local machine in order for the proper build and execution of QUASIMONT's secondary module.



# Chapter Chapter

# MODULES DESCRIPTION

In this final chapter we provide the user with a reference description for the implementation and behaviour of the methods in the source code of the library; our aim is to allow the user to better understand its features and potentially enabling an easier enhancement and/or integration in external software. The source code of each module is described in the comment block that proceeds the function definition in its source file either Datlo.cpp, MonMap.cpp or Utils.cpp (see Section 2.2). We recall that the declaration of each method can be found in the corresponding header file (located in the QUASIMONT/include subdirectory) where a comment above each method provides the "coordinates" for the user to retrieve the function description (in terms of lines and source file of reference). We divide the chapter in three sections, each one of them dedicated to the description of the methods defined in one of the three source files mentioned above. Each method is then described in the relative subsection, which takes its name. A full breakdown list of each method is reported here for reference

#### • MonMap.cpp

- computeEstimate;
- computeLambda;
- computeNumNodes;
- computeOrder;
- computeParams;
- computeQuadGl;
- computeError;

#### • DatIo.cpp

- generateTabData;
- getInputData;
- retrieveMonData;
- collectData;
- degradeData;
- exportData;

#### • Utils.cpp

- castVector;
- orderedInnerProduct;
- linspace;
- printProgress;

#### 4.1 MONMAP.CPP

#### 4.1.1 computeEstimate

```
MonMap.cpp/computeEstimate
2 //
з //
          FUNCTION: E_n = computeEstimate(lambda, n, envelope)
4 //
             INPUT: - lambda = see (18) in [1]
5 //
                   - n = see (18) in [1]
6 //
                   - envelope = string flag that specifies whether the estimate must be
7 //
8 //
                                enveloped (to avoid finite arithmetic infinities) or not
9 //
            {\tt OUTPUT: - E\_n = exact \ asymptotic \ estimate \ of \ the \ G-L \ quadrature \ error}
10 //
11 //
                     computed using (13) and (18) in [1]
12 //
       DESCRIPTION: in order for the library to generate tabulated values for
13 //
14 //
                   beta_min/beta_max as functions of n the exact estimates of the G-L
15 //
                   quadrature error must be computed with high-precision. Such an
16 //
                   a-priori estimate is generally known as results of complex analysis
17 //
                   (see [2]) however in [1] a more accurate form has been devised in
                   formulae (13) and (18) which are implemented in this routine to
18 //
19 //
                   compute the aformentioned error estimate.
20 //
         REFERENCE: [1] = Lombardi Guido - Design of quadrature rules for Muntz and
21 //
                                         Muntz-logarithmic polynomials using monomial
22 //
                                         transformation,
23 //
                                         Int. J. Numer. Meth. Engng., 80: 1687-1717,
24 //
                                         https://doi.org/10.1002/nme.2684.
25 //
                    [2] = Donaldson J.D., Elliott D. - A unified approach to quadrature
26 //
27 //
                                         rules with asymptotic estimates of their
28 //
                                         remainders.
29 //
                                         SIAM Journal on Numerical Analysis 1972;
                                         9(4):573 - 602,
30 //
31 //
                                         https://doi.org/10.1137/0709051
32 //
34
35 float1k computeEstimate(const float128& input_lambda, const int& num_nodes, const std::
     → string& envelope)
```

#### 4.1.2 computeLambda

```
MonMap.cpp/computeLambda
2 //
3 //
          FUNCTION: lambda_max = computeLambda(lambda_min, user_n)
4 //
5 //
            INPUT: - lambda_min = minimum exponent in the "muntz_sequence" input of
                    function 'getInputData'
6 //
                   - user_n = desired number of (quadrature) nodes defined by the user
7 //
8 //
9 //
            OUTPUT: - lambda_max = computed additional exponent of the polynomial
10 //
       DESCRIPTION: the monomial quadrature rule is a pre-processing of the G-L nodes \&
11 //
12 //
                   weights for those polynomials characterised by an arbitrarly large
13 //
                   gap between the terms of minimum and maximum degree. There might be
14 //
                   cases however in which the user wants to integrate singular
                   monomials; in those cases the library will require an additional,
15 //
16 //
                  non-constant, term to be added to the monomial. It does so by either
17 //
                   allowing the user to either manually input the exponent of the
18 //
                   additional term from the CLI (see lines 180~184 in the src/DatIo.cpp
                   file) or to specify the maximum number of quadrature nodes to use in
19 //
20 //
                   its application. In this last instance the the following function
21 //
                   automatically generates the resulting exponent of the additional
22 //
                   term (lambda_max).
23 //
26 float128 computeLambda(float128& lambda_min, int num_nodes)
```

#### 4.1.3 computeNumNodes

```
MonMap.cpp/computeNumNodes
2 //
3 //
          FUNCTION: n = computeNumNodes(lambda_min, lambda_max)
4 //
5 //
             INPUT: - lambda_min = minimum exponent in the input "muntz_sequence"
6 //
                     (strictly greater than -1)
7 //
                   - lambda_max = maximum exponent in the input "muntz_sequence"
8 //
9 //
            \mathtt{OUTPUT}: - n = number of (quadrature) nodes computed as solution of equation
10 //
                        (62) in [1]
11 //
       DESCRIPTION: once the exponents in the terms with minimum and maximum degree in
12 //
13 //
                   the user-input polynomial have been determined, this method
14 //
                   implements formula (62) in [1], which is a 7-th degree polynomial in
15 //
                   n, and extract its only real root whose integer floor will then be
                   the minimum possible number of (quadrature) nodes to be used in G-L
16 //
17 //
                   formula to achieve double precision (the polynomial solver itself
18 //
                   is a class method implemented in GSL-GNU Scientific Library).
19 //
         REFERENCE: [1] = Lombardi Guido - Design of quadrature rules for Muntz and
20 //
21 //
                                        {\tt Muntz-logarithmic\ polynomials\ using\ monomial}
                                        transformation,
22 //
23 //
                                        Int. J. Numer. Meth. Engng., 80: 1687-1717,
24 //
                                        \verb|https://doi.org/10.1002/nme.2684|.
25 //
28 int computeNumNodes(const float128& lambda_min, const float128& lambda_max)
```

#### 4.1.4 computeOrder

```
MonMap.cpp/computeOrder
2 //
3 //
         FUNCTION: r = computeOrder({lambda_min, lambda_max}, {beta_min, beta_max})
4 //
5 //
            INPUT: - {lambda_min, lambda_max} = output of function 'getInputData'
                  - {beta_min, beta_max} = output of function 'retrieveMonData'
6 //
7 //
8 //
           OUTPUT: - r = real value of the transformation order of the monomial map
9 //
       DESCRIPTION: the order of the monomial transformation for the new nodes and weight
10 //
11 //
                  of the G-L quadrature formula is computed as a linear interpolation
12 //
                  beetween r_min and r_max reported in (63) of [1].
13 //
        REFERENCE: [1] = Lombardi Guido - Design of quadrature rules for Muntz and
14 //
                                      Muntz-logarithmic polynomials using monomial
15 //
                                      transformation,
16 //
                                      Int. J. Numer. Meth. Engng., 80: 1687-1717,
17 //
18 //
                                      https://doi.org/10.1002/nme.2684.
19 //
21
22 double computeOrder(const std::vector<float128>& lambdas, const std::vector<double>& betas)
```

#### 4.1.5 computeParams

```
MonMap.cpp/computeParams
2 //
3 //
          FUNCTION: [J, {new_x, new_w, old_x, old_w}] = computeParams(r, n_min, I)
4 //
5 //
             INPUT: - r = output of function 'computeOrder'
6 //
                    n_min = output of function 'retrieveMonData'
7 //
                   - I = [a,b] = interval of integration of the user-input polynomial
8 //
9 //
            OUTPUT: - J = jacobian of the affine map phi: [a,b] \rightarrow [-1,1] of the G-L
10 //
                         quadrature formula
                   - {new_x, new_w} = new set of G-L quadrature nodes (x) and
11 //
12 //
                                     weights (w) following the monomial map
13 //
                   - \{old_x, old_w\} = classical set of G-L quadrature nodes (x) and
14 //
                                     weights (w) in [-1, 1]
15 //
       DESCRIPTION: once the transformation order is available, the monomial map itself
16 //
                   is constructed according to (55) in [1]; of course, prior to the
17 //
18 //
                   monomial map is applied, the G-L nodes and weights have to be mapped
                   from the user-input interval I = [a,b] to [-1, 1]. This is
19 //
                   implemented in this routine which also carries the jacobian of the
20 //
21 //
                   affine map among the outputs since it is the multiplication
                   coefficient of the integral itself (thus needed by the function
22 //
23 //
                   'computeQuadGl'). Furthermorethe classic G-L nodes and weights are
                   outputted as well so that comparisons ca be made between the
24 //
25 //
                   traditional G-L quadrature integral and the monomial rule quadrature.
26 //
28
29 std::tuple<double, std::vector<float50>, std::vector<float50>, std::vector<float50>,

→ vector <float50 >> computeParams(const double& r, const int& n_min, const std::vector <
</p>
     ⇔ double>& interval)
```

#### 4.1.6 computeQuadGl

```
MonMap.cpp/computeQuadGl
2 //
          FUNCTION: quadrature = computeQuadGl(x, w, muntz_sequence, coeff_sequence)
3 //
4 //
5 //
             INPUT: -x = G-L quadrature nodes
                   - w = G-L quadrature weights
6 //
7 //
                   - muntz_sequence = sequence of real exponents of the polynomial
8 //
                   - coeff_sequence = sequence of real coefficients of the polynomial
9 //
            OUTPUT: - quadrature = G-L quadrature of user-input polynomial
10 //
11 //
12 //
       DESCRIPTION: every interpolatory quadrature rule approximates the definite integral
13 //
                   by means of a weighted sum of the kernel's values on specific points
                   along the integration interval (i.e. nodes); an interpolatory
14 //
15 //
                   Gaussian quadrature formula is a quadrature rule whose nodes
16 //
                   corresponds to the roots of a polynomial that is orthogonal in the
17 //
                   integration interval to the weight function of the kernel. A G-L
18 //
                   quadrature formula with n+1 nodes is a Gaussian formula for which the
                   nodes corresponds to the roots of the Legendre n-th degree polynomial
19 //
20 //
                   that is orthogonal to the weight function w(x) = 1 in [-1, 1]. This
21 //
                   routine implements the G-L quadrature formula provided classical and
22 //
                   new G-L nodes and weights.
23 //
26 template < typename type >
27 type computeQuadG1(const std::vector<type>& nodes, const std::vector<type>& weights, std::
     → vector<float128>& muntz_sequence, std::vector<float128>& coeff_sequence)
```

#### 4.1.7 computeError

```
MonMap.cpp/computeError
2 //
3 //
          FUNCTION: error = computeError({post_map_quadrature, pre_map_quadrature},
4 //
                                       muntz_sequence, coeff_sequence, I)
5 //
6 //
            INPUT: - {post_map_quadrature, pre_map_quadrature} = output of function
7 //
                                                             'computeQuadGl'
8 //
                   - muntz_sequence = sequence of real exponents of the polynomial
                   - coeff_sequence = sequence of real coefficients of the polynomial
9 //
                   - I = [a,b] = interval of integration of the user-input polynomial
10 //
11 //
            OUTPUT: - error = relative error of the G-L quadrature computed with the new
12 //
                            nodes and weights
13 //
14 //
15 //
       {\tt DESCRIPTION:\ let\ I\_n\ be\ the\ numerical\ integral\ calculated\ using\ the\ G-L\ quadrature}
16 //
                   rule (outputed by function 'computeQuadG1') and I_ex be the exact
17 //
                   (analytic) value of such integral then the relative error of the
                   quadrature can be computed a-posteriori as R_n = |I_{ex} - I_n|/|I_{ex}|.
18 //
                   Such computation is implemented in this routine with the exact
19 //
20 //
                   integral being as precise as the user-input polynomial is.
21 //
24 template < typename type >
25 type computeError(const type& quadrature, std::vector<float128>& muntz_sequence, std::
     → vector <float128 >& coeff_sequence, std::vector <double >& interval)
```

#### 4.2 DATIO.CPP

#### 4.2.1 generateTabData

```
DatIo.cpp/generateTabData
2 //
з //
        FUNCTION: generateTabData()
4 //
           INPUT: no inputs
5 //
6 //
        OUTPUT: no ouptus
7 //
8 //
9 //
      DESCRIPTION: the entirety of the library relies on tabulated values of beta_min
                and beta_max for each even value of number of (quadrature) nodes
10 //
                and for this reason it is shipped with those values in the
11 //
12 //
                'data/TabulatedErrorValues.csv' file. However should the file be
                corrupted or deleted this routine, when triggere by the absence of
13 //
14 //
                the file itself, reconstructs such table from scratch.
15 //
17
18 void generateTabData()
```

#### 4.2.2 getInputData

```
DatIo.cpp/getInputData
2 //
3 //
          FUNCTION: [n, {lambda_min, lambda_max}] = getInputData(muntz_sequence,
4 //
                                                             coeff sequence)
5 //
6 //
           INPUT: - muntz_sequence = sequence of real exponents of the polynomial
7 //
                 - coeff_sequence = sequence of real coefficients of the polynomial
8 //
          OUTPUT: - n = output of function 'computeNumNodes'
9 //
10 //
                 - lambda_min = minimum exponent in the input "muntz_sequence"
11 //
                 - lambda_max = maximum exponent in the input "muntz_sequence"
12 //
13 //
       DESCRIPTION: the user-input polynomial is provided to the library via Main.cpp; the
14 //
                   polynomial itself is specified via a unordered sequence of
15 //
                   coefficients and exponents of the various monomials in the polynomial.
                   Once those input are read, checks have to be made in order to validate
16 //
17 //
                   the proper functioning of the library; those are:
18 //
                       the number of exponents and the number of coefficients coincide;
                      - the input polynomial is at least a binomial (otherwise the
19 //
                        routine further CLI user-input is required, see lines 86\ 93 in
20 //
21 //
                        the 'src/MonMap.cpp' file);
                      - lambda_min > -1 (otherwise the program exits);
22 //
23 //
                   Once those checks are ran the exponents' sequence is sorted locally
                   and lambda_min/lambda_max are thus identified and outputted alongside
24 //
25 //
                   the associated number of nodes computed by the function
                   'computeNumNodes' (see lines 110~175 in the 'src/MonMap.cpp' file).
26 //
27 //
30 std::tuple<int, std::vector<float128>> getInputData(std::vector<float128>& muntz_sequence,
     → std::vector<float128>& coeff_sequence)
```

#### 4.2.3 retrieveMonData

```
DatIo.cpp/retrieveMonbData
2 //
3 //
          FUNCTION: [n_min, {beta_min, beta_max}] = retrieveMonData(n)
4 //
5 //
          INPUT: - n = output of function 'getInputData'
6 //
7 //
          OUTPUT: - n_min = minimum possible (even) number of nodes from the
8 //
                          'data/TabulatedErrorValues.csv' file
                 - beta_min = minimum value for the exponent of the post-map polynomial
9 //
10 //
                 - beta_max = maximum value for the exponent of the post-map polynomial
11 //
12 //
       DESCRIPTION: the monomial transformation gamma: [0,1] -> [0,1] is uniquely
13 //
                   identified by its order r which in turn requires the knowledge of
14 //
                   beta_min/beta_max, alongside lambda_min/lambda_max, to be computed
15 //
                   (see lines 178^{2}11 in the 'src/MonMap.cpp' file). This method scans
                  the tabulated vales in the 'data/TabulatedErrorValues.csv' file to
16 //
17 //
                  extract the beta_min/beta_max and n_min required by the monomial
18 //
                   quadrature rule according to the specified number of nodes as either
                   computed by the function 'computeNumNodes' (see line 243) or provided
19 //
20 //
                  as user-input (see lines 168~199, 247).
21 //
24 std::tuple <int, std::vector <double >> retrieveMonData(const int& comp_num_nodes)
```

#### 4.2.4 collectData

```
DatIo.cpp/collectData
2 //
3 //
         FUNCTION: {quadratures, errors} = degradeData([J, {new_x, new_w, old_x, old_w}],
4 //
                                                 muntz_sequence, coeff_sequence)
5 //
6 //
          INPUT: - [J, {new_w, new_w, old_w, old_w}] = output of function 'computeParams'
7 //
                 muntz_sequence = sequence of real exponents of the polynomial
8 //
                - coeff_sequence = sequence of real coefficients of the polynomial
9 //
10 //
         OUTPUT: - integrals = output of function 'computeQuadGl'
11 //
                - error = output of function 'computeError'
12 //
13 //
       DESCRIPTION: due to the fact that multiple routines across the library share the
                  same inputs, a routine is implemented that collects all different
14 //
15 //
                  data-structures of those inputs and 'packages' it in a std::vector
16 //
19 std::vector <double > collectData(const std::vector <double > & interval, const std::tuple <int,

→ std::vector <float128>>& input_data, const double& transf_order)
```

#### 4.2.5 degradeData

```
DatIo.cpp/degradeData
2 //
3 //
         FUNCTION: degradeData()
4 //
5 //
            \label{eq:input: old_x, old_w} \begin{subarray}{ll} INPUT: - [J, {new_x, new_w, old_x, old_w}] = output of function \\ \end{subarray}
6 //
                                                     'computeParams'
                   - muntz_sequence = sequence of real exponents of the polynomial
7 //
8 //
                   - coeff_sequence = sequence of real coefficients of the polynomial
9 //
10 //
           OUTPUT: no outputs
11 //
12 //
       DESCRIPTION: TBA
13 //
15
16
17 void degradeData(std::tuple <double, std::vector <float50>, std::vector <float50>, std::vector
     \hookrightarrow <float50>, std::vector<float50>>& quad_params, std::vector<float128>& muntz_sequence
     → , std::vector<float128>& coeff_sequence, const std::vector<double>& collected_data)
```

#### 4.2.6 exportData

```
DatIo.cpp/exportData
2 //
          FUNCTION: exportData({lambda_min, lambda_max}, [n_min, {beta_min, beta_max}],
3 //
                              [], {post_map_integral, pre_map_integral}, r)
4 //
5 //
6 //
             INPUT: - {lambda_min, lambda_max} = output of function 'getInputData'
                    - [n_min, {beta_min, beta_max}] = output of function 'retrieveMonData'
7 //
                    - [] = output of function 'computeParams'
8 //
9 //
                    - {post_map_integral, pre_map_integral} = output of function
10 //
                                                            'computeQuadGl'
11 //
                    - r = output of function 'computeOrder'
12 //
13 //
            OUTPUT: no outputs
14 //
15 //
       DESCRIPTION: once the monomial quadrature rule is completed the resulting data is
16 //
                    streamed in output text files inside the output subdirectory created,
                    by this routine, within the calling directory of the executable of this library. The output data is splitted in three files with
17 //
18 //
                    'Results.txt' containing recap informations of the execution
19 //
                    (including the resulting integral) and 'Nodes.txt' and 'Weights.txt'
20 //
21 //
                    containg the classic and new G-L nodes and weights respectively.
22 //
25 template < typename type >
26 void exportData(const std::tuple<double, std::vector<float50>, std::vector<float50>, std::
     → vector <float50 >, std::vector <float50 >> & quad_params, const std::vector <type > &
     → output_data, const std::vector < double > & collected_data)
```

#### 4.3 UTILS.CPP

#### 4.3.1 castVector

```
Utils.cpp/castVector
з //
        FUNCTION: castVector(input_vector, output_vector)
4 //
          INPUT: - input_vector = vector of length n of type float50
5 //
                - input_vector = vector of length n of type T
6 //
7 //
8 //
          OUTPUT: no outputs
9 //
      DESCRIPTION: this method casts the float50 input vector to the an output vector
10 //
11 //
                with the same content but type T provided by the user.
12 //
15 template < typename type >
16 void castVector(const std::vector<float50>& input_vector, std::vector<type>& output_vector)
```

#### 4.3.2 orderedInnerProduct

```
Utils.cpp/orderedInnerProduct
2 //
3 //
         FUNCTION: inner_product = ordereInnerProduct(input_vector)
4 //
5 //
           INPUT: - input_vector = input vector of type float1k
6 //
7 //
           OUTPUT: - inner_product =
8 //
9 //
      DESCRIPTION: in multiple instances throughout the library, addition of terms close
10 //
                 to the format epsilon is performed (especially when computing the
11 //
                 quadrature). To avoid numeric cancellation of these terms we must
12 //
                 therefore sum those smallest values first in the highest precision
13 //
                 possible. This method takes as input the terms of the inner product
                 of the terms of two vectors of length n, sorts it in ascending order
14 //
15 //
                 and sums along n, thereby assuring that no numerical cancellation
16 //
                 occurs.
17 //
20 float1k orderedInnerProduct(std::vector<float1k>& input_vector)
```

#### 4.3.3 linspace

```
Utils.cpp/linspace
2 //
3 //
        FUNCTION: equispaced_nodes = linspace(x_0, x_m, m)
4 //
5 //
           INPUT: -x_0 = starting node (infimum)
                 x_m = ending node (supremum)
6 //
7 //
                 - m = number of sub-intervals
8 //
          OUTPUT: - equispaced_nodes = array of m+1 equispaced \langle type \rangle between x_0 and x_m
9 //
10 //
      DESCRIPTION: this method implements the linspace MATLAB function, generating a
11 //
12 //
                 linearly-spaced vector of nodes between a starting and ending point.
13 //
15
16 template < typename type >
17 std::vector<type> linspace(const type& start_type, const type& end_type, const int&
    → num_steps)
```

#### 4.3.4 printProgress

```
Utils.cpp/printProgress
2 //
3 //
        FUNCTION: printProgressBar(iterator, number_of_iterations)
4 //
          INPUT: - iterator = value of the incremending integer index in the 'for' loop
5 //
                - number_of_iterations = end-value of the iterator in the 'for' loop
6 //
7 //
8 //
         OUTPUT: no outputs
9 //
10 //
      DESCRIPTION: in a traditional for(int k=0; k < num_k; k++) this function prints a
11 //
                progress bar on the terminal line to represent the status of
12 //
                completion of the loop.
13 //
15
void printProgressBar(const int& iter, const int& num_iter)
```



### **Bibliography**

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