

The Design of Core 2: A Library for Exact Numeric Computation in Geometry and Algebra*

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Abstract. There is a growing interest in numeric-algebraic techniques in the computer algebra community as such techniques can speed up many applications. This paper is concerned with one such approach called **Exact Numeric Computation** (ENC). The ENC approach to algebraic number computation is based on iterative verified approximations, combined with constructive zero bounds. This paper describes **Core 2**, the latest version of the **Core Library**, a package designed for applications such as non-linear computational geometry. The adaptive complexity of ENC combined with filters makes such libraries practical. **Core 2** smoothly integrates our algebraic ENC subsystem with transcendental functions with ε -accurate comparisons. This paper describes how the design of **Core 2** addresses key software issues such as modularity, extensibility, and efficiency in a setting that combines algebraic and transcendental elements. Our redesign preserves the original goals of the **Core Library**, namely, to provide a simple and natural interface for ENC computation to support rapid prototyping and exploration. We present examples, experimental results, and timings for our new system, released as **Core Library 2.0**.

1 Introduction

Most algorithms involving numbers are designed in the Real RAM model of computation. In this model (e.g., [1, 37]) real numbers can be directly manipulated, comparisons are error-free, and basic arithmetic operations are exact. But

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in actual implementations, real numbers are typically approximated by machine floating point numbers, leading to the ubiquitous numerical nonrobustness issues that plague applications in scientific and engineering applications. In Computational Geometry, these numerical errors are exacerbated by the presence of discrete geometric relations defined by numbers. The survey articles [24,40] give an overview of nonrobustness issues in a geometric setting.

Now suppose P is a C++ program using only standard libraries. When compiled, it suffers from the expected nonrobustness associated with numerical errors. Imagine a software library with the property that when it is included by P , the compiled program (magically) runs like a real RAM program because all numerical quantities¹ behave like true real numbers. Such a library would be a boon towards eliminating numerical nonrobustness. The `Core Library` [22] was designed to approximate this dream: the program P only needs to insert the following two directives:

```
#define CORE_LEVEL 3
#include "CORE.h" (1)
```

Our library (`CORE.h`) will re-interpret the standard number type `double` as an `Expr` object (a directed acyclic graph representing a numerical expression). Indeed, by changing the `CORE_LEVEL` to 1 or 2 in (1), the program P can be compiled into other “accuracy levels”, corresponding to machine precision (Level 1) or arbitrary multiprecision (Level 2). Although Levels 1 and 2 fall short of a Real RAM, the ability for a single program P to compile into different accuracy levels has interesting applications in the debug-exploration-release cycle of program development [44]. The purpose of this paper is to present the rationale and design of `Core Library 2.0` (or `Core 2`). Towards this end, it will be compared to our original design, which refers to `Core Library 1.7` (or `Core 1`). Thus “old system/design” refers to `Core 1` while “new system/design” refers to `Core 2`.

§1. On implementing a Real RAM. How do we implement a Real RAM? This dream in its full generality is impossible for two fundamental reasons. First, real numbers are uncountably many while any implementation is no more powerful than Turing machines which can only access countably many reals. The second difficulty is the general impossibility of deciding zeros (equivalently, making exact comparisons) [45]. The largest class beyond algebraic zeros for which zero is decidable are the elementary constants of Richardson [38,39,45]; this result depends on the truth of Schanuel’s conjecture. What is possible, however, is to provide a Real RAM for interesting subsets of the reals. If program P uses only the rational operations (\pm, \times, \div) then such a library could be a `BigRational` number package; such a solution may have efficiency issues (e.g., [47]). If P also uses the square-root operation, then no off-the-shelf library will do; our precursor to `Core Library` [24] was designed to fill this gap. Since many basic problems

¹ We are exploiting the ability of C++ to overload operators. Otherwise, we can use some preprocessor.

in the algorithms literature involve at most irrationalities of the square-root kind, such a library is already quite useful. The natural goal of supporting all real algebraic numbers was first attained in `Core Library` 1.6 [44]. The other library that supports exact comparisons with algebraic numbers represented by floating-point approximations is `LEDA` [27, 28]. Although our algebraic number subsystem is central to our library, it is not discussed in this paper since it is not the focus of our redesign effort. Interested readers are referred to [24] which describes how we achieve Real RAM capabilities efficiently for this subsystem, using constructive root bounds and filter techniques.

Another major library that is premised on exact comparison is `CGAL` [16]. Although `CGAL` does not have its own engine for general exact algebraic computation, its generic programming design supports number kernels such as the `Core Library`. Thus `Core Library` is bundled with `CGAL`, and commercially distributed by `Geometry Factory`. In the last decade, such libraries have demonstrated that the exact comparison approach is a practical way of eliminating nonrobustness in many applications.

The computation of our algebraic program P could, in principle, be carried out by computer algebra systems (CAS). Why is there a need for something like `Core Library`? First of all, if we may use a retail business analogy, many CAS systems adopt the “department store” approach to providing services while `Core Library` takes the “boutique” approach: our main service is a number type `Expr` that allows the simulation of a Real RAM. Our system is aimed at geometric applications that have salient differences from typical CAS applications. CAS are often used for one-of-a-kind computation which might be very difficult. These computations seek to elucidate the algebraic properties of numbers while geometric applications [11, 20] are interested in their analytic properties [45]. Inputs for geometric algorithms have some combinatorial size parameter n that can be moderately large. The algebraic aspects of its computation are normally encapsulated in a handful of algebraic predicates $Q(\mathbf{x})$ (e.g., orientation predicate) or algebraic expressions $E(\mathbf{x})$ (e.g., distance between two points) where $\mathbf{x} = (x_1, \dots, x_k)$ represents the input. Evaluating $Q(\mathbf{x})$ or $E(\mathbf{x})$ is easy from the CAS viewpoint, but we must repeat this evaluation many times (as a function that grows with n). See [45, 46] for more discussion.

§2. Exact Numerical Computation. There are four ingredients in our real RAM implementation:

- (a) certified approximation of basic real functions (e.g., [4]),
- (b) the theory of constructive zero bounds [6, 29],
- (c) a precision-driven evaluation mechanism [24], and
- (d) a filter mechanism [5, 17].

The first two ingredients are essential for any Real RAM implementation; the last two ingredients are keys to making the system efficient and practical. The certified approximations in (a) are ultimately dependent on interval techniques [33]. The **constructive zero bound** in (b) is a systematic way to compute a bound $B(E)$ for a numerical expression E such that if E is defined and non-zero, then $|E| > B(E)$. Using this, we are able to do exact comparisons. We can view

(c) as a pro-active kind of lazy evaluation – this is expanded below in Section 3.3. Finally, a simplified view of “filters” in (d) is to regard them as certified machine arithmetic. Using them we can cheaply perform exact comparisons in the majority of input instances, despite the fact that exact comparisons are very difficult in the worst case. This form of computation is² characterized as **Exact Numeric Computation** (ENC) in [45,46]. Computer algebra textbooks (e.g., [9]) list several alternatives for computing with algebraic numbers; to this list, we may now add the ENC approach.

There are many libraries (e.g., [21, 31, 32, 43]) for arbitrary precision real computation. But lacking the critical ingredient (b), they cannot support exact comparison. As substitute for exact comparison, they use “ ϵ -comparison” that compares numbers up to any desired $\epsilon > 0$ accuracy. Brattka and Hertling [3] provides a theoretical study of Real RAM with ϵ -comparisons. Numerical analysts also use this ϵ -accuracy approach. In this paper, we will need to integrate an exact subsystem for algebraic numbers with a new ϵ -accurate part for transcendental numbers.

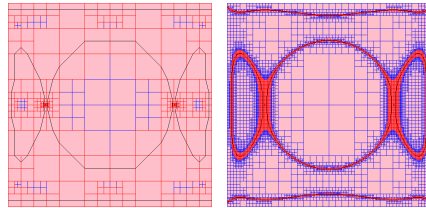


Fig. 1. Isotopic Approximation of curve $\sin_3(x^2) - \cos_3(y^2) = 0$ with **Core 2**.

As an illustration of ENC applications, Figure 1 shows the curve $f(x, y) = \sin_3(x^2) - \cos_3(y^2) = 0$ approximated by **Core 2**, using a recent algorithm [25]. Here \sin_n, \cos_n means we use the first n terms of their Taylor expansions. Our computation in the left figure stops once the isotopy-type is determined; in the right figure, we continue to a user-specified Hausdorff distance. Until recently, most exact computation on algebraic curves and surfaces are based on strong algebraic techniques such as resultant computation (e.g., [2]). In ENC, our main techniques are evaluation and domain subdivision (such subdivision boxes are seen in Figure 1). Superficially, this resembles the traditional numerical approaches, but ENC can provide the topological guarantees [25,36] that are normally only associated with algebraic algorithms. ENC algorithms have many advantages: adaptive complexity, relatively easy to implement, and locality (i.e., we can restrict computational effort to a local region, as in Figure 1).

§3. Goals of this Paper. There are three main motivations for the present redesign effort. The first is the desire to incorporate transcendental functions in

² Also known as Exact Geometric Computation (EGC) in the context of geometric applications.

our expressions. Many computations need transcendental constants (π , e , $\ln 2$, etc.) or transcendental functions ($\sin x$, $\exp x$, $\ln x$, etc.). For instance, the problem of shortest path amidst planar disc obstacles [8], or motion planning in robotics involving holonomic or dynamic constraints or helical motion are all transcendental problems. In molecular simulations where we compute Coulombic forces, we need the error function erf , which is an instance of hypergeometric functions [14, 15]. But we no longer guarantee the sign of such expressions.

The second motivation is to make the `Expr` class more flexible, extensible and modular. Although these are standard concerns of software engineering, we will discuss their special manifestations in an ENC software. There are many opportunities to introduce specialized operators into `Expr`, and we would like to introduce mechanisms to support this. Invisible to users, the evaluation of expressions relies on two critical functions: **filters** [5, 7, 17] and **zero bounds** [6, 35]. In `Core 1`, both functionalities are integrated into the `Expr` class, making them hard to maintain and extend.

The third motivation is the perpetual quest for improved efficiency. There are two major sources of inefficiency that we address. The centerpiece of any ENC library is a poly-algorithm³ to evaluate a numerical expression [24]. First, we re-examine this evaluation poly-algorithm. The optimal design of this poly-algorithm is far from understood, but we will see much room for improvement. The other efficiency issue arises in the numerical engine that delivers high precision approximations. Intuitively, this engine is a BigFloat number system combined with interval arithmetic. We will see that it plays two distinct roles but these roles are conflated in `Core 1`.

Lastly, our redesign must preserve the simple numerical API of `Core Library` as illustrated by the code snippet (1), and is thus backward compatible with `Core 1`.

§4. Overview. Section 2 reviews the original design of `Core Library` and discusses the issues. Sections 3 and 4 present (resp.) the new design of the main C++ classes for expressions and bigFloats. Section 5 describes new facilities to make `Expr` extensible. We conclude in Section 6. Many topics in this paper appear in greater detail in the Ph.D. thesis [13] of one of the authors. The source code for all experiments reported here are found in the subdirectory `progs/core2paper`, found in our open source (QPL license) `Core 2` distribution [10]. Experiments are done on an Intel Core Duo 2.4 GHz CPU with 2 GB of memory. The OS is Cygwin Platform 1.5 and compiler is `g++-3.4.4`.

2 Review of Core Library, Version 1

The `Core Library` features an object-oriented design, implemented in C++. A basic goal of the `Core Library` is to make ENC techniques transparent and

³ By a “poly-algorithm”, we mean a suite of complementary algorithms that work together to solve a specific problem.

easily accessible to (non-specialist) programmers through a simple numerical⁴ API (illustrated by (1)). User convenience is high priority because we view **Core Library** as a tool for experimentation and rapid prototyping.

There are three main subsystems in **Core 1**: the expression class (**Expr**), the real number class (**Real**) and the big float number class (**BigFloat**). These are number classes, built over standard big number classes (**BigInt**, **BigRat**) which are wrappers around corresponding types from GNU’s multiprecision package **GMP**. The **Expr** class provides the critical functionalities of ENC. In theory, **Expr** is the only number type users need, but experienced users can also access the underlying number classes directly (with `CORE_LEVEL` set to 4 in (1)). An instance of **Expr** is a directed acyclic graph (DAG) representing a numerical constant constructed from arbitrary real algebraic number constants. In the following, we raise some issues in the old design of the **Expr** and **BigFloat** classes.

- Some critical facilities in **Expr** should be modularized and made extensible. Specifically, the filter and root bound facilities have grown considerably over the course of development and are now hard to maintain, debug, or extend.
- The main evaluation algorithm (the “poly-algorithm” in the introduction) of **Expr** has three co-recursive subroutines. The old design does not separate their roles clearly, and this can lead to costly unnecessary computations.
- **Core 1** supports only algebraic expressions. An overhaul of the entire design is needed to add support for non-algebraic expressions.
- Currently, users cannot easily add new operators to **Expr**. E.g., it is useful to add diamond operator [6, 41], product, summation (see below), etc.

Next consider the **BigFloat** class. It is used by **Expr** to approximate real numbers, and is the workhorse for the library. It is implemented on top of **BigInt** from **GMP**. The old **BigFloat** is represented by a triple $\langle m, err, e \rangle$ of integers, representing the interval $[(m - err)B^e, (m + err)B^e]$ where $B = 2^{14}$ is the base. We say the bigfloat is **normalized** when $err < B$ and **exact** when $err = 0$. The following issues arise:

- The above representation of **BigFloat** has performance penalty as we must do frequent error normalization. Some applications do not need to maintain error. E.g., in self-correcting Newton-type iterations, it is not only wasteful but may fail to converge unless we zero out the error by calling `makeExact`. Users can manually call `makeExact` but this process is error-prone.
- Our **BigFloat** assumes that for exact bigfloats, the ring operations $(+, -, \times)$ are computed exactly. This is important for ENC but we see situations below where this is undesirable and the IEEE model of round-off is preferable.
- The old **BigFloat** supports only $\{+, -, *, /, \sqrt{}\}$. For **Expr** to support transcendental functions such as `exp`, `sin`, etc., we need their **BigFloat** analogues (recall ingredient (a) in ¶2). This implementation is a major effort, and the correct rounding for transcendental functions is quite non-trivial [12, 30].

⁴ API stands for “Application Programmers Interface”

To bring out these performance penalties, we compare our old `BigFloat` implementation of `sqrt` based on Newton iteration against MPFR [18]: `Core 1` was 25 times slower as seen in Figure 8. The MPFR package satisfies all three criteria above. A key feature of MPFR is its support of the IEEE rounding modes (the “R” in MPFR refers to rounding). Hence a critical decision of `Core 2` was to capitalize on MPFR.

3 Redesign of the Expr Package

We first focus on expressions. The goal is to increase modularity and extensibility of expression nodes, and also to improve efficiency.

3.1 Incorporation of Transcendental Nodes

What is involved in extending expressions to transcendental operators? In `Core 1`, we classify nodes in `Expr` into rational or irrational ones as such information is critical for root bound computation. We now classify them into `integer`, `dyadic`, `rational`, `algebraic`, and `transcendental`. A node is transcendental if any of its descendants has a transcendental operator (e.g., a leaf for $\pi = 3.1415\dots$, or a unary node such as `sin(.)`). This refined classification of nodes is exploited in root bounds. There is a natural total ordering on these types, and the type of a node is the maximum of the types in descendant nodes. As transcendental expressions do not have root bounds, we introduce a user-definable global value called `escape bound` to serve as their common root bound. Another bound called `cutoff bound` is used for a different purpose; both are explained below.

3.2 New Template-based Design of ExprRep

The `Expr` class in `Core 2` is templated, unlike in `Core 1`. It remains only a thin wrapper around a “rep class” called `ExprRep`, which is our focus here.

§5. ExprRep and ExprRepT. The filter and root bound facilities were embedded in the old `ExprRep` class. We now factor them out into two functional modules: `Filter` and `Rootbd`. The `Real` class (see Section 2), which was already an independent module, is now viewed as an instance of an abstract number module called `Kernel`. The role of `Kernel` is to provide approximate real values. We introduce the templated classes `ExprT` and `ExprRepT`, parametrized by these three modules:

```
template <typename Rootbd,
          typename Filter, typename Kernel>
class ExprT;

template <typename Rootbd,
          typename Filter, typename Kernel>
class ExprRepT;
```

Now, `Expr` and `ExprRep` are just typedefs:

```
typedef ExprT<BfmsskRootBd<BigFloat2>,
           BfsFilter<BigFloat2>, BigFloat2> Expr;
typedef ExprRepT<RootBd,
               Filter, Kernel> ExprRep;
```

The actual template arguments for `Rootbd`, `Filter`, and `Kernel` for `Expr` are passed to `ExprRep`, `ExprT`, and `ExprRepT`. The benefit of this new design is that now we can replace `Filter`, `Rootbd` or `Kernel` at the highest level without any changes in `ExprRep`, `ExprT` or `ExprRepT`. We see here that the default `Expr` class in `Core 2` uses the k-ary BFMS root bounds [6, 35] and the new `BigFloat2` kernel (below). But users are free to plug in other modules. E.g., one could substitute a better filter and root bound for division-free expressions. This design of `Expr` follows the “delegation pattern” in Object-Oriented Programming [42]: the behavior of `Expr` is delegated to other objects (filters, etc).

§6. ExprRepT class hierarchy. The class `ExprRepT` defines abstract structures and operations which are overridden by its subclasses. This hierarchy of subclasses is shown in Figure 2.

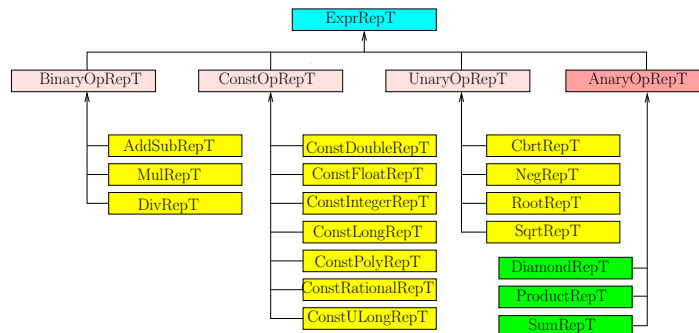


Fig. 2. `ExprRepT` Class hierarchy

There are four directly derived classes, corresponding to the arities of the operator at the root of the expressions: constants, unary, binary, and anary operators. Each of them has further derived classes – for instance, the binary operator class is further derived into three subclasses corresponding to the four arithmetic operators (`AddSubRepT`, `MulRepT`, `DivRepT`). The class `AddSubRepT` combines addition and subtraction as these two operations share basically the same code. The introduction of anary operators is new. An anary operator is one without a fixed arity, such as summation $\sum_{i=1}^n t_i$ and product $\prod_{i=1}^n t_i$. Another is the diamond operator $\diamond(a_0, \dots, a_n, i)$ to extract the i th real root of a polynomial $p(x) = \sum_{i=0}^n a_i x^i$ [6] where a_i 's are expressions. Below we show the usefulness of these extensions.

§7. Memory layout of ExprRepT. Size of expression nodes can become an issue (see Section 5). Our design of ExprRepT optimizes the use of space (see Figure 3(a)). Each ExprRepT node has three fields `_filter`, `_rootbd` and `_kernel`. Here, `_filter` is stored directly in the node, while `_rootbd` and `_kernel` are allocated on demand, and only pointers to them are stored in the node. This is because the filter computation will always be done, but root bound and high precision approximations (from `_kernel`) may not be needed. No memory will be allocated when they are not needed. The memory layout of ExprRepT is shown in Figure 3(b). E.g., a binary ExprRepT node uses a total of 48 bytes on a 32-bit architecture. The field `_cache` is added to cache important small but potentially expensive information such as `sign`, `uMSB`, `lMSB`. The field `_numType` is used for node classification.

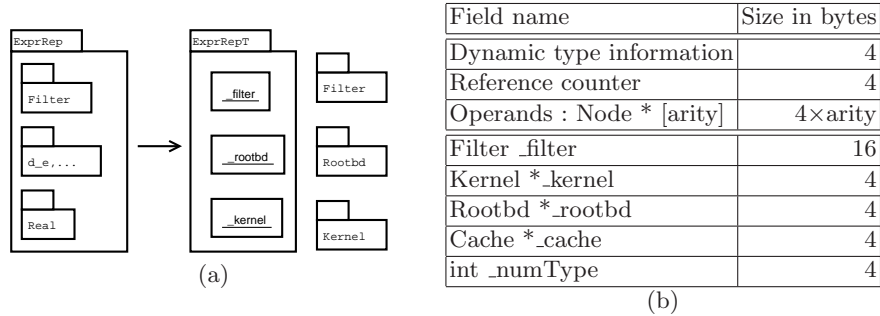


Fig. 3. (a) Comparing ExprRep and ExprRepT. (b) Layout in 32-bit architecture.

§8. Some Timings. We provide two performance indicators after the above redesign. In Figure 4(a), we measure the time to decide the sign of determinants, with and without (w/o) the filter facility, in Core 1 and Core 2. The format ‘ $N \times d \times b$ ’ in the first column indicates the number N of matrices, the dimension d of each matrix and the bit length b of each matrix entry (entries are rationals). Interestingly, for small determinants, the filtered version of Core 1 is almost twice as fast. All times are in microseconds.

MATRIX	Core 1.7 Time with (w/o) filter	Core 2.0 Time with (w/o) filter	Speedup
1000x3x10	9 (621)	19 (232)	0.5 (2.7)
1000x4x10	26 (1666)	43 (530)	0.6 (3.1)
500x5x10	449 (1728)	204 (488)	2.2 (3.5)
500x6x10	1889 (3493)	597 (894)	3.2 (3.9)
500x7x10	4443 (6597)	1426 (1580)	3.1 (4.2)
500x8x10	8100 (11367)	2658 (2820)	3.0 (4.0)

(a)

bit length L	Core 1	Core 2	Speedup
1000	0.82	0.59	1.4
2000	6.94	1.67	4.2
8000	91.9	11.63	7.9
10000	91.91	30.75	3.0

(b)

Fig. 4. (a) Timing filter facility (b) Timing root Bound facility

In Figure 4(b), we test the new root bound facility by performing the comparison $\sqrt{x} + \sqrt{y} : \sqrt{x + y + 2\sqrt{xy}}$ where x, y are b -bit rational numbers. As

this expression is identically zero, filters do not help and root bounds will always be reached.

3.3 Improved Evaluation Algorithm

Since the evaluation algorithm is the centerpiece of an ENC library, it is crucial to tune its performance.

§9. Algorithms for `sign()`, `uMSB()` and `lMSB()`. Core 1 has two main evaluation subroutines, `computeApprox()` and `computeExactSign()` (see [24]). The former computes an approximation of the current node to some given (composite) precision bound. The latter computes the sign, upper and lower bounds on the magnitude of the current node. The sign of an expression node is critical in many places. E.g., the division operator must check the sign of the right child to detect divisions by zero. But to get the sign of an expression E , we may need to estimate upper (E^+) or lower (E^-) bounds on the magnitude of the expression. These three values are maintained in `Expr` as `sign()`, `uMSB()` and `lMSB()`. In Core 1, `computeExactSign()` computes them simultaneously using the rules in Table 5.

E	Case	$E.sgn()$	E^+	E^-
Constant x		$sgn(x)$	$\lceil \log_2 x \rceil$	$\lfloor \log_2 x \rfloor$
$E_1 \pm E_2$	if $E_1.sgn() = 0$ if $E_2.sgn() = 0$ if $E_1.sgn() = \pm E_2.sgn()$ if $E_1.sgn() \neq \pm E_2.sgn()$ and $E_1^- > E_2^+$ if $E_1.sgn() \neq \pm E_2.sgn()$ and $E_1^+ < E_2^-$ otherwise	$\pm E_2.sgn()$ $E_1.sgn()$ $E_1.sgn()$ $E_1.sgn()$ $\pm E_2.sgn()$ unknown	E_2^+ E_1^+ $\max\{E_1^+, E_2^+\} + 1$ $\max\{E_1^+, E_2^+\}$ $\max\{E_1^+, E_2^+\}$ $\max\{E_1^+, E_2^+\}$	E_2^- E_1^- $\max\{E_1^-, E_2^-\}$ $E_1^- - 1$ $E_2^- - 1$ unknown
$E_1 \times E_2$		$E_1.sgn() * E_2.sgn()$	$E_1^+ + E_2^+$	$E_1^- + E_2^-$
$E_1 \div E_2$		$E_1.sgn() * E_2.sgn()$	$E_1^+ - E_2^-$	$E_1^- - E_2^+$
$\sqrt[k]{E_1}$		$E_1.sgn()$	E_1^+/k	E_1^-/k

Fig. 5. Recursive rules for computing `sign`, `uMSB`, `lMSB`.

There are two “unknown” entries in Table 5. In these cases, `computeApprox()` will loop until the sign is determined, or up to the root bound. To compute such information, we recursively compute sign and other information over the children of this node, whether needed or not. This can be unnecessarily expensive. In Core 2, we split the two routines into five co-recursive routines in `ExprRepT`: `get_sign()`, `get_uMSB()`, `get_lMSB()`, `refine()` and `get_rootBd()`. In `Expr` the corresponding methods `sign()`, `uMSB()` and `lMSB()` simply calls `get_sign()`, etc. Depending on the operator at a node, these co-routines can better decide which information from a child is really necessary. The structure of these algorithms are quite similar, so we use `get_sign()` as an example:

SIGN EVALUATION ALGORITHM, `get_sign()`:

1. Ask the filter if it knows the sign;
2. Else if the cache exists, ask if sign is cached;
Note: the cache may contain non-sign information
3. Else if the approximation (`_kernel`) exists, ask if it can give the sign;
4. Else if the virtual function `compute_sign()` returns `true`, return `sgn()` (sign is now in the cache);
5. Else call `refine()` (presented next) to get the sign.

Thus it is seen that, for efficiency, we use five levels of computation in `get_sign()`: filter, cache, kernel, recursive rules (called `compute_sign()`), and `refine()`. Note that we do not put the cache at the first level. We do not even cache the `sign`, `uMSB` and `lMSB` information when the filter succeeds because a `Cache` structure is large and we try to avoid costly memory allocation.

The object oriented paradigm used by the above design is called the “template method pattern” [19, p. 325]: define the skeleton of an algorithm in terms of abstract operations which is to be overridden by subclasses to provide concrete behavior. In the derived classes of `ExprRepT`, it is sufficient to just override the virtual function `compute_sign()` when appropriate. For example, `MulRepT` may override the default `compute_sign()` function as follows:

```

1 virtual bool compute_sign() {
2   sign() = first->get_sign() * second->get_sign();
3   return true; }

```

§10. Algorithm for `refine()`. As seen in the `get_sign()` algorithm, if the first four levels of computation fail, the ultimate fall-back for obtaining sign (and also for lower bounding magnitude) is the `refine()` algorithm. We outline this key algorithm to obtain sign via refinement:

1. If the node is transcendental, get the global escape bound. Otherwise, compute the constructive root bound.
2. Take the minimum of the bound from step 1 and the global cutoff bound.
3. Compute an initial precision. If an approximation exists, use its precision as the initial precision. Otherwise use 52 bits instead which is the relative precision that a floating-point filter can provide.
4. Initialize the current precision to the initial precision. Then enter a for-loop that doubles the current precision each time, until the current precision exceeds twice the bound computed in step 2.
5. In each iteration, call `a_approx()` (see below) to approximate the current node to an absolute error less than the current precision. If this approximation suffices to give a sign, return the sign immediately (skip the next step).
6. Upon loop termination, set the current node to be zero.
7. Check if the termination was caused by reaching the escape bound or cutoff bound. If so, append **zero assertion** to a diagnostic file in the current directory. This assertion says that “the current node is zero”.

§11. Conditional Correctness. The cutoff bound in the above `refine()` algorithm is a global variable that is set to `CORE_INFITY` by default. While escape bound affects only transcendental nodes, the cutoff bound sets an upper bound on the precision in `refine()` for all nodes. Thus it may override computed zero bounds and escape bounds. During program development, users may find it useful to set a small cutoff bound using `set_cut_off_bound()`. Thus, *our computation is correct, conditioned on the truth of all the zero assertions in the diagnostic file.*

§12. Computing Degree Bounds. In the `refine()` algorithm above, the first step is to compute a constructive root bound. Most constructive root bounds need an upper bound on the degree of an algebraic expression [24]. For radical expressions, a simple upper bound is obtained as the product of all the degrees of the radical nodes (a radical node $\sqrt[k]{E}$ has degree k). A simple recursive rule can obtain the degree bound of E from the degree bounds of its children (e.g., [23, Table 2.1]). But this bound may not be tight when the children share nodes. The only sure method is to traverse the entire DAG to compute this bound. To support this traversal, in `Core 1` we store an extra flag `visited` with each `ExprRep`. Two recursive traversals of the DAG are needed to set and to clear these flags, while computing the degree bound. To improve efficiency, we use the `std::map` (or `std::hash_map`) data structure in `STL` to compute the degree bound: we first create a map M and initialize the degree bound D to 1. We now traverse the DAG, and for each radical node u , if its address does not appear in M , we multiply its degree to the cumulative degree bound D and save its address in M . At the end we just discard the map M . This approach requires only one traversal of the DAG.

3.4 Improved Propagation of Precision

An essential feature of precision-driven evaluation is the need to propagate precision bounds [24]. Precision propagation can be illustrated as follows: if we want to evaluate an expression $z = x + y$ to p -bits of absolute precision, then we might first evaluate x and y to $(p + 1)$ -bits of absolute precision. Thus, we “propagate” the precision p at z to precision $p + 1$ at the children of z . This propagation is correct provided x and y have the same sign (otherwise, $p + 1$ bits might not suffice because of cancellation). In general, we must propagate precision from the root to the leaves of an expression. In `Core 1`, we use a pair $[a, r]$ of real numbers that we call “composite precision” bounds. If $x, \tilde{x} \in \mathbb{R}$, then we say \tilde{x} is an $[a, r]$ -**approximation** of x (written, “ $\tilde{x} \approx x[a, r]$ ”) if $|\tilde{x} - x| \leq 2^{-a}$ or $|\tilde{x} - x| \leq |x|2^{-r}$. If we set $a = \infty$ (resp., $r = \infty$), then \tilde{x} becomes a standard **relative r -bit** (resp., an **absolute a -bit**) **approximation** of x . It is known that a relative 1-bit approximation would determine the sign of x ; so relative approximation is generally infeasible without zero bounds. The propagation of composite bounds is tricky, and various small constants crop in the code, making the logic hard to understand and maintain (see [34]). Our redesign offers

a simpler and more intuitive solution in which we propagate either absolute or relative precision, not their combination.

§13. Algorithms for `r_approx()` and `a_approx()`. Core 1 has one subroutine `computeApprox()` to compute approximations; we split it into two subroutines `a_approx()` and `r_approx()`, for absolute and relative approximations (respectively). Above, we saw that `refine` calls `a_approx()`. There are two improvements over Core 1: first, propagating either absolute or relative precision is simpler and can avoid unnecessary precision conversions. Second, the new algorithms do not always compute the sign (which can be very expensive) before approximation.

§14. Overcoming inefficiencies of Computational Rings. Another issue relates to the role **computational rings** in ENC (see §16 in [45]). This is a countable set $\mathbb{F} \subseteq \mathbb{R}$ that can effectively substitute for the uncountable set of real numbers. To achieve exact computation, \mathbb{F} needs a minimal amount of algebraic structures [45]. We axiomatize \mathbb{F} to be a subring of \mathbb{R} that is dense in \mathbb{R} , with \mathbb{Z} as a subring. Furthermore, the ring operations together with division by 2, and comparisons are effective over \mathbb{F} . BigFloats with exact ring operations is a model of \mathbb{F} , but IEEE bigFloats is not. For computations that do not need exactness, the use of such rings may incur performance penalty. To demonstrate this, suppose we want to compute $\sqrt{2} \cdot \sqrt{3}$ to relative p -bits of precision. We describe two methods for this. In Method 1, we approximate $\sqrt{2}$ and $\sqrt{3}$ to relative $(p + 2)$ -bits, then perform the exact multiplication of these values. In Method 2, we proceed as in Method 1 except that the final multiplication is performed to relative $(p + 1)$ -bits. The timings (in microseconds) are shown in Figure 6. We use loops to repeat the experiment since the time for single runs is short. It is seen that Method 2 can be much more efficient; this lesson is incorporated into our refinement algorithm.

Precision	Loops	Method 1	Method 2	Speedup
10	1000000	345	191	45%
100	100000	60	46	23%
1000	10000	72	71	1%
10000	1000	267	219	18%
100000	100	859	760	12%

Fig. 6. Timing for computing $\sqrt{2} \cdot \sqrt{3}$ w/ and w/o exact multiplication.

4 Redesign of the BigFloat system

The BigFloat system is the “engine” for Expr, and Core 1 implements our own BigFloat. In Section 2, we discussed several good reasons to leverage our system on MPFR, an efficient library under active development for bigFloat numbers

with directed rounding. Our original `BigFloat` plays two roles: to implement a computational ring [45] (see section section 3.4), and to provide arbitrary precision interval arithmetic [33]. Computational ring properties are needed in exact geometry: e.g., to compute implicit curve intersections reliably, we can evaluate polynomials with exact `BigFloat` coefficients, at exact `BigFloat` values, using exact ring operations. Interval arithmetic is necessary to provide certified approximations. For efficiency, `Core 2` splits the original `BigFloat` class into two new classes: (1) A computational ring class, still called `BigFloat`. (2) An interval arithmetic class called `BigFloat2`, with each interval represented by two `MPFR` bigFloats. This explains⁵ the “2” in its name.

4.1 The BigFloat Class as Base Real Ring

The new class `BigFloat` is based on the type `mpfr_t` provided by `MPFR`. `MPFR` follows the IEEE standard for (arbitrary precision) arithmetic. The results of arithmetic operations are rounded according to user-specified output precision and rounding mode. If the result can be exactly represented, then `MPFR` always outputs this result. E.g., a call of `mpfr_mul(c, a, b, GMP_RNDN)` will compute the product of a and b , rounding to nearest `BigFloat`, and put the result into c . The user must explicitly set the precision (number of bits in the mantissa) of c before calling `mpfr_mul()`. To implement the computational ring `BigFloat`, we just need to automatically estimate this precision. E.g., we can use the following:

Lemma 1. *Let $f_i = (-1)^{s_i} \cdot m_i \cdot 2^{e_i}$ (for $i = 1, 2$) be two bigFloats in `MPFR`, where $1/2 \leq m_i < 1$ and the precision of m_i is p_i . To guarantee that all bits in the mantissa of the sum $f = f_1 \pm f_2$ is correct, it suffices to set the precision of f to*

$$\begin{cases} 1 + \max\{p_1 + \delta, p_2\} & \text{if } \delta \geq 0 \\ 1 + \max\{p_1, p_2 - \delta\} & \text{if } \delta < 0 \end{cases}$$

where $\delta = (e_1 - p_1) - (e_2 - p_2)$. Similarly, for multiplication, it suffices to set the precision of f to be $p_1 + p_2$ in computing $f = f_1 \cdot f_2$.

See [13] for a proof. While this lemma is convenient to use, it may overestimate the needed precision. In binary notation, think of the true precision of c as the minimum number of bits to store the mantissa of c . Trailing zeros in the mantissa contributes to over-estimation. To avoid this, we provide a function named `mpfr_remove_trailing_zeros()` whose role is to remove the trailing zeros. In an efficiency tradeoff, it only removes zeros by chunks (chunks are determined by `MPFR`'s representation). To understand the effect of overestimation, we conduct an experiment in which we compute the factorial $F = \prod_{i=1}^n i$ using two methods: In Method 1, we initialize $F = 1$ and build up the product in a for-loop with $i = 2, 3, \dots, n$. In the i -th loop, we increase the precision of F using Lemma 1, then call `MPFR` to multiply F and i , storing the result back into F . In Method 2, we do the same for-loop except that we call

⁵ Happily, it also coincides with the “2” in the new version number of `Core Library`.

`mpfr_remove_trailing_zeros()` on F after each multiplication in the loop. Instead of F , we can repeat the experiment with the arithmetic sum $S = \sum_{i=1}^n i$. The speedup for the second method over the first method is shown in Figure 7 (time in microseconds, precision in bits).

n	$F = \prod_{i=1}^n i$		$S = \sum_{i=1}^n i$	
	trailing zeros (prec/msec)	no zeros (prec/msec)	trailing zeros (prec/msec)	no zeros (prec/msec)
10^2	575/0	436/0	102/0	31/0
10^3	8979/0	7539/0	1002/0	31/0
10^4	123619/62	108471/47	10002/15	31/16
10^5	1568931/9219	1416270/8891	100002/437	31/110
10^6	timeout	timeout	1000002/57313	63/1078

Fig. 7. Timing for computing F and S w/ and w/o removing trailing zeros.

§15. Benchmarks of the redesigned BigFloat. By adopting MPFR, our BigFloat class gains many new functions such as `cbirt()` (cube root) and the elementary functions (`sin()`, `log()`, etc). The performance of the BigFloat is also greatly improved. We compared the performance of Core 1 and Core 2 on `sqrt()` using the following experiment: compute \sqrt{i} for $i = 2, \dots, 100$ with precision p . The timing in Figure 8 show that Core 2 is about 25 times faster, thanks purely to MPFR.

Precision	Core 1	Core 2	Speedup
1000	25	1	25
10000	716	32	22
100000	33270	1299	25

Fig. 8. Timing comparisons for `sqrt()`.

4.2 The Class BigFloat2

BigFloat2 is the second class split off from the original BigFloat. An instance of BigFloat2 is just an interval represented by a pair of bigFloat numbers. Call this the **endpoint representation** of intervals. Besides serving as numerical engine for Expr, the BigFloat2 class is also useful for various ENC applications (e.g., in meshing algorithms of the kind producing Figure 1). In Core 1, we use the **centered representation** where an interval $[a, b]$ is represented by its center $c = (a + b)/2$ and an error bound $err = (b - a)/2$, with c a bigFloat number and err a machine long. In view of the limited precision in err , it is necessary to “normalize” the representation when it gets too large. This is

one of the disadvantages of the centered representations. In the worst case, the endpoint representation can be less efficient than the centered representation by a factor of 2, both in speed and in storage. But this loss in efficiency is compensated by ease of implementation, and by sharper error bounds. It can also be beneficial in low precision computation. We note that van der Hoeven’s `Mmxlib` [43] combines the advantages of both representations by switching from the endpoint representation to the centered representation when the precision exceeds some threshold value. Since our kernel class is a template parameter, we may experiment with such an interval class in the future.

5 Extending the Expr Class

We provide facilities for adding new operators to `Expr`. `Core 2` uses such facilities to implement the standard elementary functions. Future plans include extending elementary functions to all hypergeometric functions, following the analysis in [13,14]. We give two examples of how users can use these facilities for their own needs. We refer to Zilin Du’s thesis [13] for more details about these facilities.

5.1 Summation Operation for Expr

When an `Expr` is very large, we not only lose efficiency (just to traverse the DAG) but we often run out of memory. Consider the following code to compute the harmonic series $H = \sum_{i=1}^n \frac{1}{i}$:

```
Expr harmonic(int n) {
  Expr H(0);
  for (int i=1; i<=n; ++i)
    H = H + Expr(1)/Expr(i);
  return H; }
```

1
2
3
4
5

This function builds a deep unbalanced DAG for large n . This can easily cause segmentation faults through stack overflow (column 2 in Figure 9). In ¶6, we said that `Core 2` supports a new class of **anary** (i.e., “without arity”) nodes. In particular, we implemented the `summation` and `product` operators. Using `summation`, we can rewrite the harmonic function:

```
Expr term(int i) {
  return Expr(1)/Expr(i); }
Expr harmonic(int n) {
  return summation(term, 1, n); }
```

1
2
3
4

The improvements from this new implementation are shown in Figure 9. We can now compute the harmonic series for a much larger n , and achieve a speedup as well. Similarly, the use of `product` operator leads to speed-ups.

5.2 Transcendental Constants π , e and all that

We present our *first* transcendental node π , which is a leaf node derived from `ConstRepT`:

n	Time w/o summation	Time w/ summation	Speedup
1000	24	7	3.4
10000	3931	67	58.6
100000	(segmentation fault)	752	N/A
1000000	(segmentation fault)	12260	N/A

Fig. 9. Timings for computing harmonic series $\sum_{i=1}^n \frac{1}{i}$ (in microseconds).

```

template <typename T>
class PiRepT: public ConstRepT<T> {
public:
    PiRepT() : ConstRepT<T>() {
        compute_filter();
        compute_numtype();
    }
    // functions to compute filter and number type
    void compute_filter() const {
        filter().set(
            3.1415926535897932384626433832795028F);
        /* value is not exact*/
    }
    void compute_numtype() const
    { _numType = NODE_NT.TRASCENDENTAL; }

    // virtual functions for sign, uMSB, lMSB
    virtual bool compute_sign() const
    { sign() = 1; return true; }
    virtual bool compute_uMSB() const
    { uMSB() = 2; return true; }
    virtual bool compute_lMSB() const
    { lMSB() = 1; return true; }

    // virtual functions for r-approx, a-approx
    virtual void compute_r_approx(prec_t prec) const
    { kernel().pi(prec); }
    virtual bool compute_a_approx(prec_t prec) const
    { kernel().pi(abs2rel(prec)); }
};

```

Now the new π expression is given by:

```

template <typename T>
ExprT<T> pi()
{ return new PiRepT<T>(); }

```

Note how easy it is to do this extension — it could equally be used to introduce e or $\ln 2$ or any constant, provided the kernel class knows how to approximate it. Such constants can now freely appear in an expression, and our precision-propagation mechanism can automatically approximate the expression to any desired absolute error bound. Figure 10 gives timings for π and other elementary functions after incorporation into `Expr`.

6 Conclusion

The goal of `Core Library` is to approximate the ideal real RAM. To support rapid prototyping of algorithmic ideas in geometry and algebra, ease of use and functionality is prized above sheer efficiency. With `Core 2`, we combine exact algebraic computation with transcendental functions. Our redesigned package

Precision (bits)	Expr.	Core 2	Core 1	Speedup
10,000	π	20	—	—
	$\sqrt{\pi}$	90	—	—
	e^2	80	—	—
	$\sin(0.7)$	50	1240	25
	$\cos(0.7)$	50	1230	25
	$\tan(0.7)$	110	2490	23
100,000	π	710	—	—
	$\sqrt{\pi}$	2200	—	—
	e^2	830	—	—
	$\sin(0.7)$	4780	—	—
	$\cos(0.7)$	4650	—	—
	$\tan(0.7)$	9450	—	—

Fig. 10. Transcendental Constants and Functions

is more modular, extensible, and flexible. We gained efficiency from the design and better evaluation algorithms. We adopt the highly efficient MPFR library to improve maintainability and to gain transcendental functions. Despite this overhaul, the original simple Core Numerical API is preserved.

In the transcendental aspects, we are just leveraging the speed of MPFR into our environment. What we give back is a new convenient way to access MPFR. In 2005, MPFR won the **Many Digits Competition** [26] in a field of 9 teams that included **Maple** and **Mathematica**. Their solutions are “hand-coded” in the sense that each algorithm is preceded by an error analysis to determine the needed precision, plus a hand-coded implementation of these error bounds. By incorporating MPFR into **Core 2**, we can now do these competition problems *automatically*: **Core 2** provides the automatic error analysis. Another “added value” that **Core Library** provides MPFR is access to a computational ring to support exact geometric computation. A future research is to understand and reduce any performance penalties of this automation.

A major open problem is to better understand the expression evaluation algorithms. There is no satisfactory theoretical basis for the optimal evaluation of such expressions (see some attempts in [43]). The second major problem is to provide constructive bounds for non-algebraic constants. Instead of escape bounds, we could use Richardson’s algorithm to decide zero [38, 39]. This is because all the constants in **Core 2** are elementary constants in the sense of Richardson. As Richardson suggested, this is a win-win situation because if our computation is ever wrong, we would have found a counter-example to Schanuel’s conjecture. Unfortunately, current versions of Richardson’s algorithm do not appear practical enough for general application.

Core Library represents a new breed of real number libraries to support exact numerical computation (ENC). It is made feasible through sophisticated built-in functionalities such as filters and constructive zero bounds. There remain ample opportunities for exploring the design space of constructing such libraries. Our **Core Library** offers one data point. Such libraries have many potential applications. Besides robust geometric algorithms, we can use them in geometric theorem proving, certifying numerical programs, and in mathematical explorations.

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