Correctly Rounded Arbitrary-Precision Floating-Point Summation

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Introduction to GNU MPFR

Goal: complete rewrite of the `mpfr_sum` function for the future GNU MPFR 4.

GNU MPFR in a few words:

- An efficient *multiple-precision floating-point* library with *correct rounding* (and signed zeros, infinities, NaN, and exceptions, but no subnormals).
- Radix 2. Each number has it *own precision* $\geqslant 1$ (or 2 before MPFR 4).
- 5 rounding modes: nearest-even; toward $-\infty$, $+\infty$, 0; away from zero. The functions return the sign of the error: *ternary value*.

About the GNU MPFR internals:

- Based on GNU MP, mainly the low-level *mpn* layer. A multiple-precision natural number: array of 32-bit or 64-bit integers, called *limbs*.
- Representation of a floating-point number with 3 fields: sign, significand (array of limbs, with value in $[1/2, 1[$), exponent in $[\![1 - 2^{62}, 2^{62} - 1]\!]$. Special data represented with special values in the exponent field.

`mpfr_sum`: *correctly rounded sum* of N numbers ($N \geqslant 0$).

The Old `mpfr_sum` Implementation

Demmel and Hida's accurate summation algorithm + Ziv loop.

MPFR 3.1.3 [2015-06] and earlier: `mpfr_sum` was buggy with different precisions.
Reference here: trunk r8851 / MPFR 3.1.4 [2016-03] (latest release).

Performance issues:

- The working precision must be the same for all inputs and the output.
  $\rightarrow$ The maximum precision had to be chosen as the base precision (bug fix).
- The exact result may be very close to a *breakpoint*. Uncommon case, but...
  Large exponent range $\rightarrow$ *critical issue* (e.g., crashes due to lack of memory).
- High-level for MPFR (`mpfr_add` calls). $\rightarrow$ Prevents good optimization.

Specification (behavior) issues:

- The sign of an exact zero result is not specified.
- The *ternary value* is valid only when zero is returned: for some exact results, one knows that they are exact, otherwise one has no information.

The New mpfr_sum Algorithm and Implementation

Goals:

- As fast as possible. In particular, the exponent range should no longer matter.
  $\rightarrow$ Low level (*mpn*), based on the representation of the numbers.
- Completely specified. Exact result 0: same sign as a succession of binary $+$.

Basic ideas: [r10503, 2016-06-24]

1. Handle **special inputs** (NaN, infinities, only zeros, $N_{\mathrm{regular}} \leqslant 2$). Otherwise:
2. **Single memory allocation** (stack or heap): accumulator, temporary area...
3. Fixed-point **accumulation** by blocks in some window $[\![\mathtt{minexp}, \mathtt{maxexp}[\![$ (re-iterate with a shifted window in case of cancellation): `sum_raw`.
   Done in two's complement representation.
4. If the **Table Maker's Dilemma** (TMD) occurs, then compute the sign of the error term by using the same method (`sum_raw`) in a low precision.
5. **Copy/shift** the truncated result to the destination (**normalized**).
6. **Convert** to sign $+$ magnitude, with **correction term** at the same time.

The New `mpfr_sum`: An Example

Just an example (not the common case), covering most issues (cancellations. . .).

Simplification for readability:

- Small blocks (may be impossible in practice: the accumulator size is a multiple of the limb size, i.e. 32 or 64).
- The numbers are ordered (in the algorithm, there are loops over all the numbers and the order does not matter).
- We will not show the accumulator, just what is computed at each step.

The New `mpfr_sum`: An Example [2]

`MPFR_RNDN` (roundTiesToEven), output precision `sq` $= 4$.

$N_{\mathrm{regular}} = 10$ input numbers, each with its own precision:

$$
\begin{array}{rcl}
x_0 & = & +0.1011101000010 \cdot 2^{0} \\
x_1 & = & -0.10001 \cdot 2^{0} \\
x_2 & = & -0.11000011 \cdot 2^{-2} \\
x_3 & = & -0.11101 \cdot 2^{-8} \\
x_4 & = & -0.11010 \cdot 2^{-9} \\
x_5 & = & +0.10101 \cdot 2^{-1000} \\
x_6 & = & +0.10001 \cdot 2^{-2000} \\
x_7 & = & -0.10001 \cdot 2^{-2000} \\
x_8 & = & -0.10000 \cdot 2^{-3000} \\
x_9 & = & +0.10000 \cdot 2^{-4000}
\end{array}
$$

```
+ 1011101000010
- 10001
-   11000011
-         11101
-          11010
```

The New mpfr_sum: An Example [3]

First iteration: $[\![\texttt{minexp}, \texttt{maxexp}[\![= [\![-8, 0[\![$ (maxexp: chosen from the maximum exponent; minexp: chosen from various parameters, see details later).

Only 3 input numbers are concerned:

```
              ┌─ minexp = -8
+ 10111010[00010]
- 10001
-   110000[11]
  ──────────
...000000010         (If the signs were reversed: ...111111110, e = -7)
          └─ e = -6
```

During the same loop over all the input numbers, we compute the next maxexp: Let $\mathcal{T} = \{i : Q(x_i) < \texttt{minexp}\}$, where $Q(x)$ is the exponent of the last bit of x, be the indices of the inputs that have not been fully taken into account. Then

$$\texttt{maxexp2} = \sup_{i \in \mathcal{T}} \min(E(x_i), \texttt{minexp}) = \texttt{minexp} = -8.$$

The New `mpfr_sum`: An Example [4]

We have computed an approximation to the sum and we have an error bound: $N_{\mathrm{regular}} \cdot 2^{\mathtt{maxexp2}}$, or $2^{\mathtt{err}}$ with $\mathtt{err} = \mathtt{maxexp2} + \lceil \log_2(N_{\mathrm{regular}}) \rceil$.

The accuracy test is of the form: $\mathtt{e} - \mathtt{err} \geqslant \mathtt{prec}$, where $\mathtt{prec}$ is (currently) $\mathtt{sq} + 3 = 7$. Here, $\mathtt{e} - \mathtt{err} = (-6) - (-8) - \lceil \log_2(N_{\mathrm{regular}}) \rceil \leqslant 0 < \mathtt{prec}$.
→ We need at least another iteration.

Second iteration: $[\![\mathtt{minexp}, \mathtt{maxexp}[\![= [\![-17, -8[\![$.

```
...0010             ← previous sum (shifted in the accumulator)
  +     00010
  -     11
  -     11101
  -      11010
  ______________
...0000000000000
```

Full cancellation (here with a big gap: $\mathtt{maxexp2} = -1000 \ll \mathtt{minexp}$).
→ New iteration with $\mathtt{maxexp} := \mathtt{maxexp2}$ just like in the first iteration.

The New mpfr_sum: An Example [5]

The next and last 5 input numbers:

$$\begin{aligned} x_5 &= +0.10101 \cdot 2^{-1000} \\ x_6 &= +0.10001 \cdot 2^{-2000} \\ x_7 &= -0.10001 \cdot 2^{-2000} \\ x_8 &= -0.10000 \cdot 2^{-3000} \\ x_9 &= +0.10000 \cdot 2^{-4000} \end{aligned}$$

Third iteration: $[\![\mathtt{minexp}, \mathtt{maxexp}[\![= [\![-1008, -1000[\![$.

Truncated sum $= x_5 = +0.10101 \cdot 2^{-1000}$.

$\mathtt{e} - \mathtt{err} = (-1000) - (-2000) - 4 \geqslant 7 = \mathtt{prec}$, so that the truncated sum is accurate enough, but it is close to a *breakpoint* (midpoint): TMD.

To solve the TMD:

- Do *not* increase the precision (as usually done for the elementary functions), due to potentially huge gaps (here between x_5 and x_6).
- Instead, determine the sign of the "error term" by computing this term to 1-bit target precision, using the same method ($\mathtt{prec} = 1$).

The New `mpfr_sum`: An Example [6]

The input numbers used for the error term:

$$\begin{aligned} x_6 &= +0.10001 \cdot 2^{-2000} \\ x_7 &= -0.10001 \cdot 2^{-2000} \\ x_8 &= -0.10000 \cdot 2^{-3000} \\ x_9 &= +0.10000 \cdot 2^{-4000} \end{aligned}$$

First iteration of the TMD resolution: full cancellation between x_6 and x_7.

Second iteration of the TMD resolution: x_8; accurate enough $\rightarrow$ negative.

Correctly rounded sum $= +0.1010 \cdot 2^{-1000}$.

Technical note: 2 cases to initiate the TMD resolution.

- Here, the gap between the breakpoint and the remaining bits is large enough. We start with a zeroed new accumulator.
- But a part of the error term may have already been computed in the lower part of the accumulator. In such a case, the new accumulator is initialized with some of these bits.

The New `mpfr_sum`: Accumulation (`sum_raw`)

To implement the steps presented in the example (before rounding)...

Function for accumulation: `sum_raw`

Computes a truncated sum in an accumulator such that if the exact sum is 0, return 0, otherwise satisfying $\mathtt{e} - \mathtt{err} \geqslant \mathtt{prec}$, where e is the exponent of the truncated sum.

Calls of `sum_raw`:

- Main approximation: $\mathtt{prec} = \mathtt{sq} + 3$; zeroed accumulator in input.
- TMD resolution, if necessary: $\mathtt{prec} = 1$ (only the sign of the result is needed); the accumulator may be zeroed or initialized with some of the lowest bits from the main approximation.

The New `mpfr_sum`: Accumulation (`sum_raw`) [2]

The accumulator, for the first iteration:

- cq $= \lceil \log_2(N_{\mathrm{regular}}) \rceil + 1$ bits for the sign bit and to avoid overflows.
- sq bits: output precision.
- dq $\geqslant \lceil \log_2(N_{\mathrm{regular}}) \rceil + 2$ bits to take into account truncation errors.

Example of first iteration and after a partial cancellation ($\rightarrow$ shift):

```
              [--------]-----------------------------------]
                  cq    ├─ maxexp     sq + dq      minexp ─┤
Before shift: 00000000000000000000000000001----------------]
              <--- identical bits (0) --->
                                  <------- 26 zeros ------->
After shift:  001-----------------00000000000000000000000000
This iteration:          minexp ─┘    ├─ maxexp2           │
Next iteration:                       └─ maxexp    minexp ─┘
```

maxexp2: maximum exponent of the *tails* (`MPFR_EXP_MIN` if no tails).

The New `mpfr_sum`: Correction (in short)

We now have 3 terms: the sq-bit truncated significand S, a trailing term t in the accumulator such that $0 \leqslant t < 1\,\mathrm{ulp}$, and an error on the trailing term.

$\rightarrow$ The error ε on S is of the form: $-2^{-3}\,\mathrm{ulp} \leqslant \varepsilon < (1+2^{-3})\,\mathrm{ulp}$.

4 correction cases, depending on ε (from t and possibly a TMD resolution), the sign of the significand, the rounding bit, and the rounding mode:

$$\mathtt{corr} = \begin{cases} -1: & \text{equivalent to nextDown} \\ 0: & \text{no correction} \\ +1: & \text{equivalent to nextUp} \\ +2: & \text{equivalent to 2 consecutive nextUp} \end{cases}$$

This is done *efficiently* with:

- For $\mathtt{sq} \geqslant 2$, one-pass operation on the two's complement significand:
  - For positive results: $x + \mathtt{corr}$.
  - For negative results: $\overline{x} + (1 - \mathtt{corr})$.

  In case of change of binade, just set the MSB to 1 and correct the exponent.
- For $\mathtt{sq} = 1$, specific code (but trivial).

Tests

Tests needed to detect various possible issues:

- unnoticed error in the pen-and-paper proof (complex due to many cases);
- coding error, such as typos (without a full formal proof of MPFR);
- bug in MPFR, such as internal utility macros (this did happen: r9295);
- bug in compilers;

and to check that some bounds in the pen-and-paper proof are optimal.

Different kinds of tests, including:

- Special values (e.g., with combinations of NaN, infinities and zeroes).
- Specific tests to trigger particular cases in the implementation. Comparison with the sum computed exactly with `mpfr_add` then rounded.
- Generic random tests with cancellations (no full check, though).
- Tests with underflows and overflows.
- Check for value coverage in the TMD cases to make sure that the various combinations have occurred in the tests (this could be improved).

Timings

Comparison of 3 algorithms:

- sum_old: mpfr_sum from MPFR 3.1.4 (old algo).
- sum_new: mpfr_sum from the trunk patched for MPFR 3.1.4 (new algo).
- sum_add: basic sum implementation with mpfr_add (inaccurate and sensitive to the order of the inputs).

Random inputs with various sets of parameters:

- array size $\mathtt{n} = 10^1$, 10^3 or 10^5;
- small or large input precision precx (the same one);
- small or large output precision precy;
- inputs uniformly distributed in $[-1, 1]$, or with scaling by a uniform distribution of the exponents in $[\![0, 10^8[\![$;
- partial cancellation or not.

Timings [2]

Inaccurate timings (up to a factor 3 between two calls), but we focus on much larger factors (theoretically unbounded).

Conclusion:

- `sum_new` vs `sum_add`:
  - sometimes slower, due to the accuracy requirements;
  - sometimes faster, as low level and low significant bits may be ignored.
- `sum_new` vs `sum_old`:
  - much faster in most cases;
  - much slower in some pathological cases: `precy` $\ll$ `precx` and there is a cancellation, due to the fact that the reiterations are always done in a low precision (assuming that a reiteration would stop with a large probability). Change in the future?

Sources and results are provided in the MPFR repository:

`https://gforge.inria.fr/scm/viewvc.php/mpfr/misc/sum-timings/`

Conclusion and Future Work

Major improvements over the old algorithm and implementation:

- Much faster in most tested cases (application dependent, though).
- Much less memory in some cases (no more crashes in simple cases).
- Fully specified, with ternary value (as usual).

Temporary memory: twice the output precision + a few limbs.

For the next MPFR release: GNU MPFR 4.0.

Possible future work:

- Determine a worst-case time complexity (could be pessimistic).
- Bad cases could be improved, but this could slow down the average case.
- What is the average case? Too much context dependent.
  $\rightarrow$ Based on real-world applications?