On the robustness of the 2Sum and Fast2Sum algorithms

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- Kahan/Dekker and Møller/Knuth;
- used (implicitely or explicitely) in most compensated algorithms (such as compensated summation, dot product or polynomial evaluation), for manipulating Floating-Point expansions, etc.
- presented assuming round-to-nearest (RN), and no overflow;
- much more robust than usually believed: the result makes sense even when the rounding function is not RN, and they are *almost* immune to overflow.

In the following program S2 is an estimate of the error caused when S = T was last rounded or truncated, and is used in statement 13 to compensate for that error. The parentheses in statement 23 must not be omitted; they cause the difference (S-T)to be evaluated first and hence, in most cases, without error because the difference is normalized before it is rounded or truncated.

$$\begin{array}{cccc} 1 & S = 0.0 \\ & S2 = 0.0 \\ 2 & DO \ 4 \ I = 1, \ N \\ 3 & YI = \cdots \\ 13 & S2 = S2 + \ YI \\ & T = S + S2 \\ 23 & S2 = (S - T) + \ S2 \\ 4 & S = T \\ 5 & \cdots \\ 5 & \cdots \end{array}$$

Until double-precision arithmetic was made a standard feature of the FORTRAN language, the author and his students used this trick on a 7090 in FORTRAN II programs to perform quadrature, solve differential equations and sum infinite series.

- Kahan, Comm. ACM, Jan. 1965;
- error of the addition $S + S_2$, re-injected in the calculation.

First appearance of Twosum

QUASI DOUBLE-PRECISION IN FLOATING POINT ADDITION 43

and making allowance for the specific treatment of $abs(v) \leq \frac{1}{2}E_u$ as e.g. takes place in the GIER computer, we conclude that provided $|v| \leq |u|$ c gives the exact correction sought for except in the following special cases:

- al $u: 10.0000 \sim -2$ and $-E_u < v < -\frac{1}{2}E_u$ (consequently lev(s) > lev(u)) causing the error to be the last figure of v.
- a2 u: 01.11..1xx..x1

 $v: 00.00..011..11x_1x_2x_3...x_f$ (and consequently lev(s)>lev(u)) in which cases the last figure of v, x_f (subf for finis), is lost.

Even more briefly we can state that in the rare cases in which Process A is incorrect the error is a cut away of the last figure of v and will never exceed $\frac{1}{2}E_{w}$. And when the error equals $\frac{1}{2}E_{u}$ the result is equivalent to using no Process A (c=0), i.e. we never do things worse than the bare addition s := u + v.

It should be noticed that only when lev(s) > lev(u) and combination \bigcirc III or IV occurs need we evaluate eu; in all other cases c := ev is sufficient.

The process could be put in a compact form by writing

$$s := u + v;$$

 $c := (v - (s - u)) + (u - (s - (s - u)))$

For the sake of completeness we shall present an extension of (3) which masters cases a1, a2.

What we do is to evaluate vlabi := v - (v1 + ev) (vlabi for last bit of v) and add this quantity to c:

$$c := ev + eu + vlabi;$$

• Møller, Quasi double-precision in floating-point addition, BIT, 1965;

• *c* is the error of the addition s := u + v.

Error of a FP addition

- barring overflow, the error of a rounded-to-nearest FP addition or subtraction *is a FPN;*
- RN is necessary: radix-2, precision-*p*, rounding toward $-\infty$, if a = 1 and $b = -2^{-3p}$, then

$$s = \text{RD}(a+b) = 0.$$
 111111...11 $p = 1 - 2^{-p},$

and

 \rightarrow cannot be exactly represented with precision *p*.

And yet...

- directed rounding functions are very useful (upper/lower bounds, stochastic arithmetic);
- a piece of code designed with RN in mind may be used in another context, willingly or not;
- furthermore,

Let a and b be binary, precision-p, FPNs. Let $s \in {\text{RD}(a+b), \text{RU}(a+b)}$. *If* $|e_a - e_b| \le p - 1$, *then* s - (a+b) *is a binary, precision-p, FPN.*

- even when the error of + is not a FPN, can we get a good approximation to that error ? Would frequently suffice;
- partial answers: Demmel & Nguyen; Graillat, Jézéquel, & Picot (Fast2Sum), Martin-Dorel et al. (RN with possible double roundings);
- can we have spurious overflows ?

Some notation

- radix-2, precision-*p*, FP arithmetic, of extremal exponents e_{\min} and e_{\max} (set F_p);
- $\Omega =$ largest representable FPN:

$$\Omega = (2 - 2^{1-p}) \cdot 2^{e_{\max}}.$$

FP predecessor and successor of *x*: pred(*x*) and succ(*x*);
if *x* ∈ ℝ, 2^k ≤ |*x*| < 2^{k+1},

$$ulp(x) = 2^{\max(k, e_{\min}) - p + 1}.$$

- rounding functions RN, RD, RU, RZ (for RN the choice of the tie-breaking rule is not important);
- the FP number \hat{x} is a faithful rounding of $x \in \mathbb{R}$ if $\hat{x} \in \{\text{RD}(x), \text{RU}(x)\}.$

Definition 1 (Rounding function—"optimal rounding" in [Kulisch71])

Function \circ from \mathbb{R} to F_p is a rounding function if

Remark 2

If \circ *is a rounding function, then for any* x, $\circ(x) \in \{ RD(x), RU(x) \}$ *.*

Introduced by Dekker in 1971 (yet used by Kahan in 1965).

Algorithm 1: Conventional Fast2Sum Algorithm.

1: $s \leftarrow \text{RN}(a + b)$ 2: $z \leftarrow \text{RN}(s - a)$ 3: $t \leftarrow \text{RN}(b - z)$

In the absence of overflow, if the radix of the FP system is ≤ 3 , and if the FP exponents e_a and e_b of a and b satisfy $e_a \geq e_b$, then

s+t=a+b.

TwoSum

Knuth (1969?) transforms Møller' trick (1965) into a Theorem.

Algorithm 2: Conventional 2Sum algorithm.

1: $s \leftarrow \text{RN}(a + b)$ 2: $a' \leftarrow \text{RN}(s - b)$ 3: $b' \leftarrow \text{RN}(s - a')$ 4: $\delta_a \leftarrow \text{RN}(a - a')$ 5: $\delta_b \leftarrow \text{RN}(b - b')$ 6: $t \leftarrow \text{RN}(\delta_a + \delta_b)$

In the absence of overflow,

s + t = a + b.

Without knowing the respective orders of magnitude of *a* & *b*, calling 2Sum in general more efficient than comparing them, swapping them if needed, and calling Fast2Sum.

S. Boldo, S. Graillat, J.-M. Muller

Theorem 3 (Hauser)

If x and y are radix- β FP numbers, and if the number RN(x + y) is subnormal, then x + y is a FP number (so that $\circ(x + y) = x + y$ for any rounding function).

Proof. *x* and *y* are multiples of the smallest nonzero FPN $\alpha = \beta^{e_{\min}-p+1} \rightarrow x + y$ is a multiple of α . If it is in the subnormal range, then it is $\langle \beta^{e_{\min}} \Rightarrow$ exactly representable.

What we are going to discuss...

Algorithm 3: Fast2Sum with faithful roundings: $\circ_1, \circ_2, \circ_3$ are rounding functions.

1: $s \leftarrow \circ_1(a+b)$ 2: $z \leftarrow \circ_2(s-a)$ 3: $t \leftarrow \circ_3(b-z)$

Algorithm 4: 2Sum with faithful roundings: \circ_i , for i = 1, ..., 6, are rounding functions.

1:
$$s \leftarrow \circ_1(a+b)$$

2: $a' \leftarrow \circ_2(s-b)$
3: $b' \leftarrow \circ_3(s-a')$
4: $\delta_a \leftarrow \circ_4(a-a')$
5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

Lemma 4 (Sterbenz)

If x and y are finite floating-point numbers such that

$$\frac{y}{2} \le x \le 2y,$$

then x - y is a FP number.

Lemma 5

Let *a* and *b* be two binary FPN of exponents e_a and e_b . Let $s \in {\text{RD}(a + b), \text{RU}(a + b)}$. If the exponent e_s of *s* is $\leq \min(e_a, e_b)$ then s = a + b.

Proof. *a* and *b* are multiple of 2^{e_a-p+1} and 2^{e_b-p+1} , respectively. Since $e_s \leq \min(e_a, e_b)$, a + b is a multiple of 2^{e_s-p+1} . By rounding it (through any rounding function) to a multiple of 2^{e_s-p+1} we just get it.

Accuracy of Fast2Sum assuming no overflow

1:
$$s \leftarrow \circ_1(a+b)$$

2: $z \leftarrow \circ_2(s-a)$
3: $t \leftarrow \circ_3(b-z)$

Lemma 6

Let a and b be two binary FPNs, with $e_a \ge e_b$. Let $s \in {\text{RD}(a+b), \text{RU}(a+b)}$. The number s - a is a FP number (\rightarrow computed exactly, with any rounding function).

Proof. Adaptation of Dekker's original proof. If $|b| \le |a|$ the proof becomes straightforward: assuming $a \ge 0$ (symmetry), we have $-a \le b \le a$, and

- if $-a \le b \le -a/2$ then Sterbenz $\Rightarrow s = a + b \Rightarrow s a = b$ is a FPN;
- if $-a/2 \le b \le a$ then $a/2 \le a + b \le 2a$ hence $a/2 \le s \le 2a \Rightarrow s a$ is aFPN.

Accuracy of Fast2Sum assuming no overflow

1:
$$s \leftarrow \circ_1(a+b)$$

2: $z \leftarrow \circ_2(s-a)$
3: $t \leftarrow \circ_3(b-z)$

Lemma 6 only holds in radix 2. **Example:** In radix 3 with p = 4 and $\circ_i = \text{RU}$, if $a = 1002_3 = 29_{10}$ and $b = 2222_3 = 80_{10}$, then

 $s = \mathrm{RU}(a+b) = 11010_3 = 111_{10},$

so that $s - a = 10001_3 = 82_{10}$ is not exactly representable with precision 4.

Accuracy of Fast2Sum assuming no overflow

1:
$$s \leftarrow \circ_1(a+b)$$

2: $z \leftarrow \circ_2(s-a) = s-a$
3: $t \leftarrow \circ_3(b-z) = \circ_3(b-(s-a)) = \circ_3((a+b)-s)$

Theorem 7

If no overflow occurs, and $e_a \ge e_b$ *then the values s and t returned by Algorithm 3 satisfy*

$$t = \circ_3((a+b)-s),$$

i.e., *t* is a faithful rounding of the error of the FP addition $s \leftarrow \circ_1(a + b)$.

 \rightarrow if the difference of the exponents of *a* and *b* does not exceed p - 1 (will occur in many practical cases), then t = (a + b) - s.

2Sum: more tricky...

1: $s \leftarrow \circ_1(a+b)$ 2: $a' \leftarrow \circ_2(s-b)$ 3: $b' \leftarrow \circ_3(s-a')$ 4: $\delta_a \leftarrow \circ_4(a-a')$ 5: $\delta_b \leftarrow \circ_5(b-b')$ 6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

t not always faithful rounding of (a + b) - s: $p = 24, a = 3076485 \cdot 2^{-21}, b = -6130317 \cdot 2^{-49},$ $\circ_1 = \circ_2 = \circ_5 = \text{RU}, \circ_3 = \circ_4 = \circ_6 = \text{RD}, \text{gives}$

$$\begin{array}{rcl} s & = & a = 3076485 \cdot 2^{-21} \rightarrow (a+b) - s = b; \\ t & = & -1532579 \cdot 2^{-47}; \end{array}$$

With any rounding function \circ , $\circ((a + b) - s) = b \neq t$. However, $(a + b - s) - t = -2^{-49} \rightarrow t$ remains a very good approximation to (a + b) - s.

2Sum: more tricky...

1: $s \leftarrow \circ_1(a+b)$ 2: $a' \leftarrow \circ_2(s-b)$ 3: $b' \leftarrow \circ_3(s-a')$ 4: $\delta_a \leftarrow \circ_4(a-a')$ 5: $\delta_b \leftarrow \circ_5(b-b')$ 6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

Theorem 8

If $p \ge 4$ *and no overflow occurs, then s and t satisfy*

 $t = (a+b) - s + \alpha,$

with $|\alpha| < 2^{-p+1} \cdot \operatorname{ulp}(a+b) \le 2^{-p+1} \cdot \operatorname{ulp}(s)$. Furthermore, if e_s and e_b satisfy $e_s - e_b \le p - 1$ then t is a faithful rounding of (a+b) - s.

Case splitting based on the location of *b*



1: $s \leftarrow \circ_1(a+b)$ 2: $a' \leftarrow \circ_2(s-b)$ 3: $b' \leftarrow \circ_3(s-a')$ 4: $\delta_a \leftarrow \circ_4(a-a')$ 5: $\delta_b \leftarrow \circ_5(b-b')$ 6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

 $|b| \ge a \Rightarrow$ lines (1), (2), and (4) of Algorithm 4 are Fast2Sum(b,a).

 \rightarrow we have a' = s - b and $\delta_a = \circ_4(a + b - s)$. An immediate consequence of a' = s - b is b' = b and $\delta_b = 0$. From this, we find

 $t = \circ_4(a+b-s)$

A straightforward case: $-a < b \le -a/2$



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3: $b' \leftarrow \circ_3(s-a')$
4: $\delta_a \leftarrow \circ_4(a-a')$
5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

Sterbenz Lemma $\rightarrow s = a + b$. Successively implies a' = a, b' = b, $\delta_a = \delta_b = t = 0$, so that

t = (a+b) - s.

We are left with the painful part: -a/2 < b < a



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5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

Let $u = 2^{1-p}$. We have

$$s = (a+b) \cdot (1+\epsilon_1); \text{ with } |\epsilon_1| \le u;$$

$$a' = (s-b) \cdot (1+\epsilon_2); \text{ with } |\epsilon_2| \le u.$$

$$\rightarrow a' = (a + a\epsilon_1 + b\epsilon_1) \cdot (1 + \epsilon_2).$$

 $|b| < a \rightarrow a\epsilon_1 + b\epsilon_1 = 2a\epsilon_3$, with $|\epsilon_3| \le u$. Therefore $a' = a \cdot (1 + \eta)$, with $|\eta| \le 3u + 2u^2$. As soon as $p \ge 4$, $|\eta| < 1/2$ so that $a/2 \le a' \le 2a \rightarrow \delta_a = a - a'$ by Sterbenz Lemma.

We are left with the painful part: -a/2 < b < a

1:
$$s \leftarrow \circ_1(a+b)$$

2: $a' \leftarrow \circ_2(s-b)$
3: $b' \leftarrow \circ_3(s-a')$
4: $\delta_a \leftarrow \circ_4(a-a') = a-a'$
5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

 $s \ge |b| \rightarrow$ Lines (2), (3), and (5) are equivalent to Fast2Sum(s, -b), so that

$$b' = s - a',\tag{1}$$

and

$$\delta_b = \circ_5(a' - (s - b)). \tag{2}$$

If $e_s - e_b \le p - 1$, then (2) implies $\delta_b = a' - (s - b)$, from which we deduce $t = \circ_6(a + b - s)$.

We are left with -a/2 < b < a and $e_s - e_b \ge p$

1:
$$s \leftarrow \circ_1(a + b)$$

2: $a' \leftarrow \circ_2(s - b)$
3: $b' \leftarrow \circ_3(s - a') = s - a'$
4: $\delta_a \leftarrow \circ_4(a - a') = a - a'$
5: $\delta_b \leftarrow \circ_5(b - b')$
6: $t \leftarrow \circ_6(\delta_a + \delta_b)$

 $e_s - e_b \ge p \Rightarrow |b| < ulp(s) \Rightarrow a' \in {succ(s), s, pred(s), pred(pred(s))},$ and the case a' = pred(pred(s)) can occur only when *s* is a power of 2.



On the robustness of 2Sum & Fast2Sum



We are left with -a/2 < b < a and $e_s - e_b \ge p$

1:
$$s \leftarrow \circ_1(a+b)$$

2: $a' \leftarrow \circ_2(s-b)$
3: $b' \leftarrow \circ_3(s-a') = s-a'$
4: $\delta_a \leftarrow \circ_4(a-a') = a-a'$
5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a + \delta_b)$

Remember: $a' \in {succ(s), s, pred(s), pred(pred(s))},$

- If $\mathbf{a}' = \mathbf{s}$ then b' = 0. It follows that $\delta_b = b$ and $\delta_a = a s$, for which we deduce $t = \circ_6(a + b s)$,
- **2** If $\mathbf{a}' \neq \mathbf{s}$ then

$$a' = s - \sigma \cdot ulp(s)$$
, with $\sigma \in \{-1, +1/2, +1\}$,

and we have

$$b' = \sigma \cdot ulp(s); \delta_a = a - s + \sigma \cdot ulp(s); \text{ and } \delta_b = \circ_5(b - \sigma \cdot ulp(s)).$$

$-a/2 < b < a, e_s - e_b \ge p$, and $a' = s - \sigma \cdot ulp(s)$

1:
$$s \leftarrow \circ_1(a + b)$$

2: $a' \leftarrow \circ_2(s - b) = s - \sigma \cdot \operatorname{ulp}(s)$
3: $b' \leftarrow \circ_3(s - a') = s - a' = \sigma \cdot \operatorname{ulp}(s)$
4: $\delta_a \leftarrow \circ_4(a - a') = a - a'$
5: $\delta_b \leftarrow \circ_5(b - b') = \circ_5(b - \sigma \cdot \operatorname{ulp}(s))$
6: $t \leftarrow \circ_6(\delta_a + \delta_b)$

Remember: |b| < ulp(s). Furthermore, *b* has the same sign as σ . Therefore

• either $|b| \ge |\sigma|/2 \cdot \text{ulp}(s)$, in which case Sterbenz Lemma $\rightarrow \delta_b = b - \sigma \cdot \text{ulp}(s) \Rightarrow \delta_a + \delta_b = a + b - s \Rightarrow t = \circ_6(a + b - s)$

• or $|b| < |\sigma|/2 \cdot ulp(s)$, in which case, from

 $|b - \sigma \cdot \mathbf{ulp}(s)| < |\sigma| \cdot \mathbf{ulp}(s)$

(unless b = 0 but that case is straightforwardly handled), we get (since $|\sigma| \cdot ulp(s)$ is a power of 2),

$$|\delta_b - (b - \sigma \cdot \mathbf{ulp}(s))| < \frac{1}{2}\mathbf{ulp}(\sigma \cdot \mathbf{ulp}(s)) = \frac{|\sigma|}{2}\mathbf{ulp}(\mathbf{ulp}(s)) = |\sigma| \cdot 2^{-p}\mathbf{ulp}(s)$$

$$-a/2 < b < a, e_s - e_b \ge p$$
, and $a' = s - \sigma \cdot ulp(s)$

1:
$$s \leftarrow \circ_1(a+b)$$

2: $a' \leftarrow \circ_2(s-b) = s - \sigma \cdot \operatorname{ulp}(s)$
3: $b' \leftarrow \circ_3(s-a') = s - a' = \sigma \cdot \operatorname{ulp}(s)$
4: $\delta_a \leftarrow \circ_4(a-a') = a - a'$
5: $\delta_b \leftarrow \circ_5(b-b') = \circ_5(b - \sigma \cdot \operatorname{ulp}(s))$
6: $t \leftarrow \circ_6(\delta_a + \delta_b)$

Consequence:

$$\begin{aligned} |(\delta_a + \delta_b) - (a + b - s)| &< |\sigma| \cdot 2^{-p} \mathrm{ulp}(s).\\ |\delta_a + \delta_b| &< \mathrm{ulp}(a + b) + |\sigma| \cdot 2^{-p} \mathrm{ulp}(s). \end{aligned}$$
(3)

• show that $\delta_a + \delta_b$ is a multiple of $|\sigma| \cdot 2^{-p} \operatorname{ulp}(s) \rightarrow |\delta_a + \delta_b| < \operatorname{ulp}(a+b);$

• case splitting (is *s* a power of 2?, is it above or below a + b?)

$$\rightarrow |t - (a+b-s)| < 2^{-p+1} \mathrm{ulp}(a+b).$$

Fast2Sum is immune to overflow

1:
$$s \leftarrow \circ_1(a+b)$$
 reminder: $e_a \ge e_b$
2: $z \leftarrow \circ_2(s-a)$
3: $t \leftarrow \circ_3(b-z)$

- assume no overflow at line 1;
- without l.o.g., assume *a* > 0;
- $s = a + b + \epsilon$, with $|\epsilon| < ulp(a + b) \le 2ulp(a)$, hence

 $s - a = b + \epsilon$

- therefore, if line (2) overflows then b < −Ω + 2ulp(a) or b > Ω − 2ulp(a)
 - if $b < -\Omega + 2ulp(a)$ then $b < -\Omega + 2ulp(\Omega)$ and (since $e_a \ge e_b$), $\Omega/2 < 2^{e_{\max}} \le a \le \Omega$. Sterbenz Lemma $\rightarrow s = a + b \rightarrow z = b \rightarrow$ no overflow at line 2;
 - if $b > \Omega 2ulp(a)$ is impossible: this and $e_a \ge e_b$ imply $a + b > \Omega/2 + \Omega 2ulp(\Omega) \rightarrow line 1$ overflows.
 - \rightarrow Line 2 cannot overflow.

1:
$$s \leftarrow \circ_1(a+b)$$

2: $z \leftarrow \circ_2(s-a)$ no overflow $\rightarrow z = s - a$
3: $t \leftarrow \circ_3(b-z)$

Line 3?

Since line 2 does not overflow, z = s - a. Hence b - z = (a + b) - s, hence

$$|b-z| < |(a+b)-s| < ulp(s) < |s|$$

 \rightarrow no overflow.

Theorem 9

Assuming $e_a \ge e_b$, if the computation of s (first line of Fast2Sum) does not overflow, then the other lines cannot overflow.

Of course, with 2Sum it is more tricky

1:
$$s \leftarrow \circ_1(a+b)$$

2: $a' \leftarrow \circ_2(s-b)$
3: $b' \leftarrow \circ_3(s-a')$
4: $\delta_a \leftarrow \circ_4(a-a')$
5: $\delta_b \leftarrow \circ_5(b-b')$
6: $t \leftarrow \circ_6(\delta_a+\delta_b)$

Theorem 10

If $|a| < \Omega$ and if there is no overflow at line (1) of the algorithm, then there will be no overflow at lines (2) to (6).

Condition $|a| < \Omega$ is necessary. Assume all rounding functions are RN (ties-to-even). The choice $a = \Omega$ and $b = -(3/2) \cdot ulp(\Omega)$ gives no overflow at line (1), and an overflow at line (2).

On the list stds-754@IEEE.ORG

De: Jason Riedy <jason.riedy@cc.gatech.edu> Objet: Updated twoSum proposal Date: 18 mai 2016 17:15:58 UTC+2

Attached is an updated twoSum proposal that provides more thorough justification for exceptional behavior. There also is some example C code for context, although that code ignores the rounding mode.

PROPOSAL: TWOSUM OPERATION Jason Riedy

Table of Contents

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.. 2.1 Properties of an existing software implementation

De: Jason Riedy <jason.riedy@cc.gatech.edu> Objet: Updated twoSum proposal Date: 18 mai 2016 20:11:35 UTC+2

And Jean-Michel Muller writes:

> That analyses the behaviour of these algorithms with various rounding modes, and shows that they are rather immune from spurious overflow.

Thank you. My "careful" version fail with your example. augh I'll work on that.

In binary FP arithmetic, 2Sum and Fast2Sum are more "robust" than it is usually believed:

- even when the error of the initial FP addition is not a FP number, they return a very good approximation to that error (→ can be used in many compensated algorithms);
- Fast2Sum totally immune to overflow;
- 2Sum almost totally immune to overflow: the only case where a "spurious" overflow may occur is when the absolute value of *a* is equal to Ω.