#### Floating-point arithmetic and error analysis (AFAE)

## Multiprecision and Interval Arithmetic

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Lecture Master 2 SFPN - MAIN5





## Outline

Interval analysis and self-validating methods

Multiple precision arithmetic

## Outline

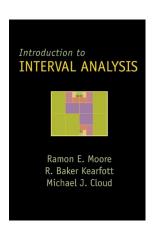
Interval analysis and self-validating methods

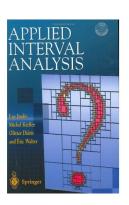
Multiple precision arithmetic

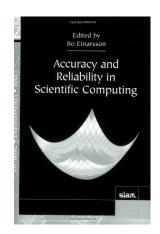
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- R. Moore, R. Kearfott et M. Cloud Introduction to Interval Analysis. SIAM, 2009
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## References







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#### Historical remarks

#### Who invented Interval Arithmetic?

- Ramon Moore in 1962 1966 ?
- T. Sunaga in 1958 ?
- Rosalind Cecil Young in 1931 ?

Cf. http://www.cs.utep.edu/interval-comp/

Popularization in the 1980, German school (U. Kulisch).

IEEE-754 standard for floating-point arithmetic in 1985: directed roundings are standardized and available.

Since the nineties: interval algorithms.

# Directed roundings

Let

$$\mathbf{x}_1 = \nabla(1/3), \quad \mathbf{x}_2 = \Delta(1/3)$$

Then we mathematically have

$$x_1 \le 1/3 \le x_2$$
 with  $x_1, x_2 \in \mathbb{F}$ 

More general  $a, b \in \mathbb{F}$ , we have :

$$\nabla(\mathbf{a} \circ \mathbf{b}) \leq \mathbf{a} \circ \mathbf{b} \leq \Delta(\mathbf{a} \circ \mathbf{b})$$

for 
$$\circ \in \{+,-,\times,/\}$$

# Directed roundings (cont'd)

#### With INTLAB

```
setround(-1) rounding downwards
setround(1) rounding upwards
setround(0) rounding to nearest
```

#### Example:

```
setround(-1)
x = 1/3
setround(1)
y = 1/3
```

Then we have the mathematical inequality

$$x \leq 1/3 \leq y$$

#### Interval arithmetic

- Interval arithmetic: replace numbers by intervals and compute.
- Fundamental theorem of interval arithmetic: the exact result belongs to the computed interval.
- No result is lost, the computed interval is guaranteed to contain every possible result.

#### Interval arithmetic

Interval Arithmetic and validated scientific computing: two directions

- replace floating-point arithmetic by interval arithmetic to bound from above roundoff errors;
- replace floating-point arithmetic and algorithms by interval ones to compute guaranteed enclosures.

#### Interval arithmetic

Interval arithmetic: replace numbers by intervals and compute.

Initially introduced to take into account roundoff errors (Moore 1966) and also uncertainties (on the physical data, etc.), then computations with sets.

Interval analysis: develop algorithms for reliable (or verified, or guaranteed) computing, that are suited for interval arithmetic,

i.e. different from the algorithms from classical numerical analysis.

## Examples of applications

- control the roundoff errors, cf. computational geometry
- solve several problems with verified solutions: linear and nonlinear systems of equations and inequations, constraints satisfaction, (non/convex, un/constrained) global optimization, etc.
- mathematical proofs: cf. Hales' proof of the Kepler's conjecture

## Definitions and notation

#### Objects

- ullet interval of real numbers: closed connected sets of  ${\mathbb R}$ 
  - interval for π: [3.14159, 3.14160]
  - data d known with absolute uncertainty of  $\varepsilon$ :  $[d-\varepsilon,d+\varepsilon]$
- interval vector

$$\mathbf{v} = \left( \begin{array}{c} [1,2] \\ [2,4] \end{array} \right)$$

interval matrix

$$\mathbf{A} = \begin{pmatrix} [1,3] & [3,4] \\ [2,5] & [1,2] \end{pmatrix}$$

Representation inf-sup of intervals

$$\mathbf{x} = [\underline{\mathbf{x}}; \overline{\mathbf{x}}] = \{\mathbf{x} \in \mathbb{R} : \underline{\mathbf{x}} \le \mathbf{x} \le \overline{\mathbf{x}}\}.$$

The set of interval of  $\mathbb{R}$  is denoted  $\mathbb{IR}$ .

## Definitions (2/3)

Representation inf-sup of intervals

$$\mathbf{x} = [\underline{\mathbf{x}}; \overline{\mathbf{x}}] = {\mathbf{x} \in \mathbb{R} : \underline{\mathbf{x}} \le \mathbf{x} \le \overline{\mathbf{x}}}.$$

- A real number is represented by [x; x].
- Interval quantities are generally represented in boldface.
- ullet The set of interval of  $\mathbb R$  is denoted  $\mathbb R$ .
- We denote by mid(x) the midpoint of an interval  $x = [\underline{x}; \overline{x}]$ ,

$$mid(\mathbf{x}) = (\overline{\mathbf{x}} + \mathbf{x})/2,$$

and by w(x) the width of x,

$$\mathbf{w}(\mathbf{x}) = \overline{\mathbf{x}} - \underline{\mathbf{x}}.$$

## Operations on intervals

Given two intervals **x**, **y** and  $\diamond \in \{+, -, \times, /\}$ , one defines

$$\boldsymbol{x} \diamond \boldsymbol{y} = \{\boldsymbol{x} \diamond \boldsymbol{y} : \boldsymbol{x} \in \ \boldsymbol{x}, \boldsymbol{y} \in \ \boldsymbol{y}\}.$$

On can implement these operations as :

$$\begin{array}{lll} \textbf{x}+\textbf{y} &=& [\underline{\textbf{x}}+\underline{\textbf{y}};\overline{\textbf{x}}+\overline{\textbf{y}}],\\ \textbf{x}-\textbf{y} &=& [\underline{\textbf{x}}-\overline{\textbf{y}};\overline{\textbf{x}}-\underline{\textbf{y}}],\\ \textbf{x}\times\textbf{y} &=& [\min\{\underline{\textbf{x}}\underline{\textbf{y}},\underline{\textbf{x}}\overline{\textbf{y}},\overline{\textbf{x}}\underline{\textbf{y}},\overline{\textbf{x}}\overline{\textbf{y}}\};\max\{\underline{\textbf{x}}\underline{\textbf{y}},\underline{\textbf{x}}\overline{\textbf{y}},\overline{\textbf{x}}\underline{\textbf{y}},\overline{\textbf{x}}\overline{\textbf{y}}\}],\\ \textbf{x}^2 &=& [\min(\underline{\textbf{x}}^2,\overline{\textbf{x}}^2),\max(\underline{\textbf{x}}^2,\overline{\textbf{x}}^2)] \text{ if } 0\notin[\underline{\textbf{x}},\overline{\textbf{x}}],\\ & [0,\max(\underline{\textbf{x}}^2,\overline{\textbf{x}}^2)] \text{ otherwise},\\ 1/\textbf{x} &=& [1/\overline{\textbf{x}};1/\underline{\textbf{x}}] \text{ if } 0\notin[\underline{\textbf{x}},\overline{\textbf{x}}],\\ \textbf{x}/\textbf{y} &=& \textbf{x}\times1/\textbf{y} \text{ if } 0\notin[\underline{\textbf{y}},\overline{\textbf{y}}],\\ \sqrt{\textbf{x}} &=& [\sqrt{\underline{\textbf{x}}},\sqrt{\overline{\textbf{x}}}] \text{ if } 0\leq\underline{\textbf{x}},\\ & [0,\sqrt{\overline{\textbf{x}}}] \text{ otherwise}. \end{array}$$

# Operations on intervals

In floating-point arithmetic, if one wants validated results, one need to take into account rounding errors!

$$\mathbf{x} + \mathbf{y} = [\nabla(\underline{\mathbf{x}} + \underline{\mathbf{y}}), \Delta(\overline{\mathbf{x}} + \overline{\mathbf{y}})] \supseteq \{\mathbf{x} + \mathbf{y} | \mathbf{x} \in \mathbf{x}, \mathbf{y} \in \mathbf{y}\}$$

$$\mathbf{x} - \mathbf{y} = [\nabla(\underline{\mathbf{x}} - \overline{\mathbf{y}}), \Delta(\overline{\mathbf{x}} - \mathbf{y})] \supseteq \{\mathbf{x} - \mathbf{y} | \mathbf{x} \in \mathbf{x}, \mathbf{y} \in \mathbf{y}\}$$

where  $\nabla$  (resp.  $\Delta$ ) representes rounding toward  $-\infty$  (resp. rounding toward  $+\infty$ ).

# Operations on intervals (cont'd)

Algebraic properties : associativity and commutativity still hold

But other properties have been lost :

- the subtraction is not the inverse of addition :  $\mathbf{x} \mathbf{x} \neq [0]$
- the division is not the inverse of multiplication
- ...

## Intervals and functions

Definition: an interval extension f of f must satisfy

$$\forall x, f(x) \subseteq f(x) \text{ et } \forall x, f(\{x\}) = f(\{x\})$$

Elementary functions:

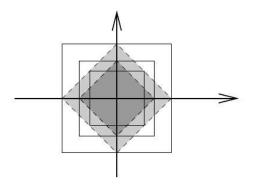
$$\exp \mathbf{x} = [\exp \underline{\mathbf{x}}, \exp \overline{\mathbf{x}}]$$
  
 $\sin[\pi/6, 2\pi/3] = [1/2, 1]$ 

# Problem: data dependency

$$x - x = \{x - y : x \in x, y \in x\} \neq \{0\}$$

# Problem: wrapping effect

Effect of 2 rotations of  $\pi/4$ 



#### Libraries

Libraries for scientific software:

- INTLAB for MATLAB/Octave;
- Mathematica;
- intpakX for Maple.

Well-know libraries integrating interval arithmetic for classic languages:

- XSC (eXtended Scientific Computing);
- "range" arithmetic;
- MPFI (Multiple Precision Floating-point Interval arithmetics library).

Computation of  $\sqrt{2}$  by Newton iteration with solving the equation f(x) = 0 with  $f(x) = x^2 - 2$ .

Newton iteration:  $x_{k+1} = x_k - (x_{\nu}^2 - 2)/(2x_k)$ 

>> x=1; for i=1:5,  $x = x - (x^2-2)/(2*x)$ . end x = 1.500000000000000x = 1.416666666666667x = 1.414215686274510

> x = 1.414213562374690x = 1 414213562373095

#### Naive interval Newton iteration starting with [1.4, 1.5]

```
>> X=infsup(1.4,1.5);
>> for i=1:5, X = X - (X^2-2)/(2*X), end
intval X =
[ 1.3107, 1.5143]
intval X =
[ 1.1989, 1.6218]
intval X =
[ 0.9359, 1.8565]
intval X =
[ 0.1632, 2.4569]
int.val X =
[-12.2002, 8.5014]
```

Problem: data dependency

Instead of an inclusion of

$$\{x-(x^2-2)/(2x):x\in X_k\},$$

naive interval arithmetic computes an inclusion of

$$\{\xi_1 - (\xi_2^2 - 2)/(2\xi_3) : \xi_1, \xi_2, \xi_3 \in \textbf{X}_k\}$$

#### **Theorem**

Let a differentiable function  $f: \mathbb{R} \to \mathbb{R}$ ,  $X = [x_1, x_2] \in \mathbb{IR}$  and  $\widetilde{x} \in X$  be given, and suppose  $0 \notin f'(X)$ . Using interval operations, define

$$N(\widetilde{x}, X) := \widetilde{x} - f(\widetilde{x})/f'(X).$$

If  $N(\widetilde{x}, X) \subset X$ , then X contains a unique root of f. If  $N(\widetilde{x}, X) \cap X = \emptyset$  then  $f(x) \neq 0$  for all  $x \in X$ .

#### Proof:

If  $N(\widetilde{\mathbf{x}},\mathbf{X}) \subset \mathbf{X}$  then  $\mathbf{x}_1 \leq \widetilde{\mathbf{x}} - f(\widetilde{\mathbf{x}})/f'(\xi) \leq \mathbf{x}_2$  for all  $\xi \in \mathbf{X}$ . Therefore  $0 \notin f'(\mathbf{X})$  implies

$$(f(\widetilde{x}) + f'(\xi_1)(x_1 - \widetilde{x})) \cdot (f(\widetilde{x}) + f'(\xi_2)(x_2 - \widetilde{x})) \leq 0$$

for all  $\xi_1, \xi_2 \in X$  and in particular  $f(x_1) \cdot f(x_2) \le 0$ .

So there is a root of f in X, which is unique because  $0 \notin f'(X)$ .

Suppose  $\hat{x} \in X$  is a root f.

By the Mean Value Theorem, there exists  $\xi \in X$  with  $f(\widetilde{x}) = f'(\xi)(\widetilde{x} - \widehat{x})$ .

So 
$$\widehat{x} = \widetilde{x} - f(\widetilde{x})/f'(\xi)$$
.

The assumptions of the Theorem are verified as follows.

- Let F and Fs be interval extensions of f and f', respectively.
- ② If Fs(X) does not contain zero 0, then  $f'(x) \neq 0$  for  $x \in X$ .
- $\textbf{ 3} \ \ \, \textbf{If} \ \, \widetilde{\textbf{x}} \textbf{F}(\widetilde{\textbf{x}})/\textbf{Fs}(\textbf{X}) \subset \textbf{X} \ \, \textbf{then} \ \, \textbf{X} \ \, \textbf{contains} \ \, \textbf{a} \ \, \textbf{unique roots of f.}$

# Proving that a matrix is nonsingular

#### **Theorem**

Let A be a matrix and R another matrix such that  $\|\mathbf{I} - \mathbf{R}\mathbf{A}\| < 1$ . Then A is nonsingular

#### Proof.

By contrapositive, if A is singular, there exists  $x\neq 0$  such that Ax=0. Then (I-RA)x=x and so  $\|I-RA\|\geq 1$ .

On a computer, choose for  $R \approx A^{-1}$  and then compute  $\|I - RA\|$  with interval arithmetic.

# Proving that a matrix is nonsingular with INTLAB

#### Let A be a matrix of dimension n

```
R = inv(A)
C = eye(n) - R*intval(A)
nonsingular = ( norm(C,1) < 1 )</pre>
```

If nonsingular = 1, then A is nonsingular.

If nonsingular = 0, then we can say nothing

## A simple approach

Let  $f: \mathbb{R}^n \to \mathbb{R}^n$  and  $\widehat{\mathbf{x}} \in \mathbb{R}^n$  unknown such that  $f(\widehat{\mathbf{x}}) = 0$ 

Let  $\widetilde{x} \approx \widehat{x}$  such that  $f(\widetilde{x}) \approx 0$ 

Find a bound for  $\tilde{x}$ : an interval X such that  $\hat{x} \in X$ 

We have

$$f(x) = 0$$
  $\Leftrightarrow$   $g(x) = x$ 

with g(x) := x - Rf(x) with  $det(R) \neq 0$ .

## Theorem (Brouwer, 1912)

Every continuous function from a closed ball of a Euclidean space to itself has a fixed point.

## A simple approach (cont'd)

By Brouwer fixed point theorem,

$$X \in \mathbb{IR}^n$$
,  $g(X) \subseteq X \Rightarrow \exists \widehat{x} \in X$ ,  $g(\widehat{x}) = \widehat{x} \Rightarrow f(\widehat{x}) = 0$ 

We just have to check  $g(X) \subseteq X$  and prove  $det(R) \neq 0$ .

But naive approach fails:

$$g(X) \subseteq X - Rf(X) \nsubseteq X$$

## Bounds for the solution of nonlinear systems

#### Mean Value Theorem:

if 
$$f \in \mathcal{C}^1$$
 then  $f(x) = f(\widetilde{x}) + M(x - \widetilde{x})$  with  $M = (\frac{\partial f}{\partial x}(\xi_i))_i$ 

Let  $Y := X - \widetilde{x}$  and

As a consequence

$$-Rf(\widetilde{x}) + (I - RM)Y \subset Y \Rightarrow q(X) - \widetilde{x} \subset Y \Rightarrow q(X) \subset X$$

## Bounds for the solution of nonlinear systems

#### **Theorem**

Let  $f: \mathbb{R}^n \to \mathbb{R}^n$  with  $f = (f_1, \dots, f_n) \in \mathcal{C}^1$ ,  $\widetilde{x} \in \mathbb{R}^n$ ,  $X \in \mathbb{R}^n$  with  $0 \in X$  and  $R \in \mathbb{R}^{n \times n}$  be given. Let  $M \in \mathbb{IR}^{n \times n}$  be given such that

$$\{\nabla f_i(\zeta):\zeta\in\ \widetilde{x}+X\}\subseteq M_{i,:}\ .$$

Assume

$$-Rf(\widetilde{x}) + (I - RM)X \subseteq int(X).$$

Then there is a unique  $\widehat{x} \in \widetilde{x} + X$  with  $f(\widehat{x}) = 0$ . Moreover, every matrix  $\widetilde{M} \in M$  is nonsingular. In particular, the Jacobian  $J_f(\widehat{x}) = \frac{\partial f}{\partial x}(\widehat{x})$  is nonsingular.

## Verification of multiple roots

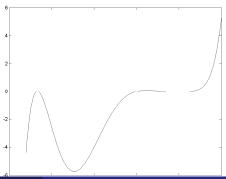
- Verification method for computing guaranteed (real or complex) error bounds for double roots of systems of nonlinear equations.
- To circumvent the problem of ill-posedness we prove that a slightly perturbed system of nonlinear equations has a double root.
- For example, for a given univariate function  $f: \mathbb{R} \to \mathbb{R}$  we compute two intervals  $X, E \subseteq \mathbb{R}$  with the property that there exists  $\widehat{x} \in X$  and  $\widehat{e} \in E$  such that  $\widehat{x}$  is a double root of  $\overline{f}(x) := f(x) \widehat{e}$ .

# Verification of multiple roots

The typical scenario in the univariate case is a function  $f : \mathbb{R} \to \mathbb{R}$  with a double root  $\widehat{x}$ , i.e.  $f(\widehat{x}) = f'(\widehat{x}) = 0$  and  $f''(\widehat{x}) \neq 0$ .

Consider, for example,

$$f(x) = 18x^7 - 183x^6 + 764x^5 - 1675x^4 + 2040x^3 - 1336x^2 + 416x - 48$$
$$= (3x - 1)^2 (2x - 3)(x - 2)^4$$



S. Graillat (SU)

### Verification of multiple roots

- Verification methods for multiple roots of polynomials already exist. A set containing k roots of a polynomial is computed, but no information on the true multiplicity can be given.
- Algorithm verifypoly in INTLAB. Computing inclusions X1, X2 and X3 of the simple root  $x_1 = 1.5$ , the double root  $x_2 = 1/3$  and the quadruple root  $x_3 = 2$  of f:

## Verification of multiple roots (cont'd)

- The accuracy of the inclusion of the double root  $x_2 = 1/3$  is much less than that of the simple root  $x_1 = 1.5$ , and this is typical.
- Perturb f into  $\widetilde{f}(x) := f(x) \varepsilon$  for some small real constant  $\varepsilon$  and look at a perturbed root  $\widetilde{f}(\widehat{x} + h)$  of  $\widetilde{f}$ , then

$$0 = \widetilde{f}(\widehat{x} + h) = -\epsilon + \frac{1}{2}f''(\widehat{x})h^2 + \mathcal{O}(h^3)$$

implies

$$h \sim \sqrt{2\epsilon/f''(\widehat{x})}$$
.

• A relative error of size  $\varepsilon \approx 10^{-16}$  implies a relative accuracy of  $\sqrt{\epsilon} \approx 10^{-8}$ .

### Dealing with double roots

• We consider for a double root the nonlinear system  $G:\mathbb{R}^2 \to \mathbb{R}$  with

$$G(x, e) = \begin{pmatrix} f(x) - e \\ f'(x) \end{pmatrix} = 0$$

in the two unknowns x and e.

• The Jacobian of this system is

$$\mathbf{J}_{G}(\textbf{x},\textbf{e}) = \left( \begin{array}{cc} f'(\textbf{x}) & -1 \\ f''(\textbf{x}) & 0 \end{array} \right) \ ,$$

so that the nonlinear system is well-conditioned for the double root  $x_2 = 1/3$  of f.

### Dealing with double roots (cont'd)

• We provide an algorithm verifynlss in INTLAB.

#### Outline

Interval analysis and self-validating methods

Multiple precision arithmetic

# The number of correct digits of a computed result

"Rule of thumb":

forward error ≈ condition number × backward error

number of correct digits

Number of correct digits =  $-\log_{10}$  (forward error)

# The number of correct digits of a computed result

Problem : determination of a multiple root  $x_*$  of multiplicity m of a polynomial  $p(x) = \sum_{i=0}^n a_i x^i$ .

A relative perturbation of u on a leads to a perturbation

$$x_*(u) - x_* = u^{1/m} \left[ -\frac{m! a_i x_*^i}{p^{(m)}(x_*)} \right]^{1/m}$$

Multiple roots : always ill-conditioned, forward error of order  $\mathbf{u}^{1/m}$ 

#### Multiple precision vs arbitrary precision

#### Arbitrary precision

used for integer or rational arithmetic, where the representation sizes of the operands vary arbitrarily and can be arbitrarily large.

#### Multiple precision

used for floating-point arithmetic, where the lengths of the mantissas and exponents are fixed but can be arbitrarily large.

#### **Applications**

Either a bit more accuracy than floating-point computations, and thus a bit more computing precision (several hundreds of bits)

or extreme computations, such as

- ullet the computation of the largest number of digits of  $\pi$ ,
- checking some special cases to prove theorems,
- determining a counter-example to a conjecture.

### Representation: with integers

A multiple-precision floating-point number is a number of the form

$$s.m.\beta^e$$
.

The mantissa (of arbitrary length) is represented as an exact integer.

Exact integers may be represented as a sequence of machine integers (cf. GMP):

$$m = \sum_{i=0}^{n} m_i B^i,$$

where  $m_i$  are machine integers and B is the length of a machine word.

#### Representation: expansions

Representation using floating-point numbers: non-evaluated sum of floating-point numbers

$$\sum_{i=0}^n\,f_i$$

where the  $f_i$  are floating-point numbers, if possible with exponents sufficiently wide apart so that the mantissas do not overlap.

#### Multiple precision libraries

 Multiple precision libraries with multiple-digit format: a number is expressed as a sequence of digits coupled with a single exponent

```
MPFR: www.mpfr.org/
ARPREC: crd.lbl.gov/~dhbailey/mpdist/
GMP: gmplib.org/
```

 Fixed precision libraries using a multiple-component format with a limited numbers of components Classic example is double-double (a double-double is a non-evaluated sum of 2 doubles)

```
DD : crd.lbl.gov/~dhbailey/mpdist/
QD : crd.lbl.gov/~dhbailey/mpdist/
```

#### Multiple precision libraries

 Multiple precision libraries using a multiple-component format where a number is expressed as unevaluated sums of ordinary floating-point words.

Shewchuk: http://www.cs.cmu.edu/~quake/robust.html
Priest

#### double-double library

A double-double number is a non-evaluated pair  $(a_h, a_l)$  of IEEE 754 floating-point numbers satisfying  $a = a_h + a_l$  et  $|a_l| \le u|a_h|$ .

## Algorithm (Addition of a double b and a double-double $(a_h, a_l)$ )

```
function [c_h, c_l] = \text{add\_dd\_d}(a_h, a_l, b)

[t_h, t_l] = \text{TwoSum}(a_h, b)

[c_h, c_l] = \text{FastTwoSum}(t_h, (t_l \oplus a_l))
```

#### double-double library

## Algorithm (Product of a double-double $(a_h,a_l)$ by a double b)

```
\begin{aligned} & \text{function } [c_h, c_l] = \text{prod\_dd\_d}(a_h, a_l, b) \\ & [s_h, s_l] = \text{TwoProduct}(a_h, b) \\ & [t_h, t_l] = \text{FastTwoSum}(s_h, (a_l \otimes b)) \\ & [c_h, c_l] = \text{FastTwoSum}(t_h, (t_l \oplus s_l)) \end{aligned}
```

#### double-double library

## Algorithm (Addition of a double-double $(a_h, a_l)$ with a double-double $(b_h, b_l)$ )

```
\begin{aligned} & \text{function } [c_h, c_l] = \text{add\_dd\_dd}(a_h, a_l, b_h, b_l) \\ & [s_h, s_l] = \text{TwoSum}(a_h, b_h) \\ & [t_h, t_l] = \text{TwoSum}(a_l, b_l) \\ & [t_h, s_l] = \text{FastTwoSum}(s_h, (s_l \oplus t_h)) \\ & [c_h, c_l] = \text{FastTwoSum}(t_h, (t_l \oplus s_l)) \end{aligned}
```

If a, b are double-double and  $\odot \in \{+, \times\}$ , then we have

$$fl(a \odot b) = (1 + \delta)(a \odot b),$$

with  $|\delta| \le 4 \cdot 2^{-106}$ .

#### Kulisch accumulator

Computing without error due to the limited range of floating-point numbers

		emax	<b>2</b> n	emin	
g	2emax		2n	2 emin	

In double precision, n = 53 bits, emin = -1022, emax = 1023 and k = 92 bits

A register of length L=k+2emax+2|emin|+2n=4288 bits is sufficient (67 words of 64 bits)

#### Kulisch accumulator

