INTERVAL COMPUTATIONS WITH INTLAB *

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Abstract. Version 5 and following of the widely used interactive programming environment Matlab supports an operator concept. This offers the possibility of easy and user-friendly access to interval operations, automatic differentiation and much more. For the toolbox INTLAB, entirely written in Matlab, new concepts have been developed for very fast execution of interval operations to be used together with the operator concept in Matlab. The new implementation of interval arithmetic is strongly based on the use of BLAS routines. Some of the new concepts are presented as well as reasoning for the very good performance.

1. Introduction. At a first glance it seems to be impossible to realize an operator concept in Matlab. This is because one of the main principles in Matlab is that *no* type declarations of variables are necessary but, by the interpretation principle, variables are automatically declared when used. Also, there is no distinction between scalars, vectors and matrices, whether they are real or complex. A variable may even frequently change its type, like in the following (artificially) constructed example:

```
for n=1:10
   if odd(n)
     A = sqrt(-n)
   else
     A = rand(n)
   end
 end
```

The variable A changes its type from complex scalar to a real matrix (of different dimension) during execution of the for-loop.

The identification of new data types in Matlab works as follows. To define a new type, say TYPE, together with operators working on it, a subdirectory with name @TYPE is to be defined. This subdirectory has to be adjacent to the search path, i.e. the parent directory of @TYPE is in the search path of Matlab, whereas the subdirectory @TYPE itself is not in the search path.

Within the subdirectory @TYPE there has to be a routine named TYPE. This is the constructor for the new data type. The core of that routine, eig. for TYPE being `intval`, could look as follows:

```
function A = intval(a)
  A.inf = a;
  A.sup = a;
  A = class(A,'intval')
```

and many more. The main statement is the last "class-constructor", which tells the Matlab system that the output is a variable of type "`intval`". From now on things are standard. Every operation involving a variable of the new data type calls the corresponding function in the subdirectory @TYPE, in our example `intval`, with fixed naming conventions. For example, names of operators are

```
+          plus
.*         times
*          mtimes
^          mpower
[ ... ]    horzcat
```

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and many more. The operator concepts also includes a user-defined display routine. For example, the statement

```
A = intval(3.5);
5+A
```

calls the `intval` constructor in the first line: The variable A is now of type `intval`. The second statement calls the function plus for arguments 5 and A, and subsequently the `intval` display routine is called because the result of $5 + A$ is of type `intval`.

Summarizing this is a really nice and easy way to define and to use new operators in Matlab. For further information see [6].

2. Performance issues. The nice working in Matlab is, there may be a severe penalty when using low-level operators. Matlab is a *Mat*rix *Lab*oratory, and extensive use of scalar operators causes much computing time due to interpretation overhead. Consider the following four ways of writing a matrix multiplication in Matlab, timing for multiplication of two randomly generated 200×200 matrices included.

```
n = 200; A = rand(n); B = rand(n);

C = zeros(n);
tic
  for i=1:n
    for j=1:n
      for k=1:n
        C(i,j) = C(i,j) + A(i,k)*B(k,j);
      end
    end
  end
toc

C = zeros(n);
tic
  for i=1:n
    for j=1:n
      C(i,j) = C(i,j) + A(i,:)*B(:,j);
    end
  end
toc

C = zeros(n);
tic
  for i=1:n
    C(i,:) = C(i,:) + A(i,:)*B;
  end
toc

C = zeros(n);
tic
  C = A*B;
toc
```

The following table for a 300 MHz Pentium I Laptop shows the interpretation overhead.

	3 loops	2 loops	1 loop	no loop
time [sec]	104.2	2.7	0.14	0.046

TABLE 2.1. *Interpretation overhead*

The table clearly shows that minimization of interpretation overhead is mandatory if the system shall not be restricted to toy problems. Consider interval matrix multiplication as our model problem.

The problem is, however, that current implementations of interval matrix operations use a top-down 3-loop approach, similar to the first one presented before. According to the above table this is much too slow in an interpretative system. However, even when using programming languages with highly optimized compilers such as Fortran or C, this top-down approach is very expensive in terms of computing time: The most inner loop is an interval operation, thus contataining if-statements and case-distinctions. Such code can barly be optimized by a compiler.

The effect of lack of optimization, of different sequence of the loops and more subtle methods like unrolled loops shall be demonstrated in the following. We restrict ourselve to pure floating point computations, no additional slow-down by interval computations present.

The first experiment is a scalar product $c = x^T y$ for $x, y \in \mathbb{R}^n$ for dimension $n = 1000$. The traditional loop is compared to an unrolled loop with five terms:

```
for ( i=0, c=0; i<n; i++)
  c += x[i]*y[i] + x[i+1]*y[i+1] + x[i+2]*y[i+2] +  \
       x[i+3]*y[i+3] + x[i+4]*y[i+4];
```

The achieved performance rates in Mflops for the standard loop and the unrolled loop, both without and with compiler optimization on a RS 6000 workstation are as follows.

Performance [Mflop]	standard loop	unrolled loop
w/o optimization	4.3	6.9
with optimization	12.7	19.9

We see quite some increase in performance by the unrolled loops and, as we expect, by the optimization of the compiler. Both is *not* possible for the standard implementation of interval matrix multiplication; in other words, performance is basically limited to the smallest number in the above table.

Another standard method for improving performance is the sequence of loops in matrix multiplication. Any of the six possibilities ijk, ikj, ..., kji computes the correct matrix product, however, with quite different performance. The following table shows performance for the six possibilities, both without and with compiler optimization.

Performance [Mflop]	jki	kji	ikj	kij	ijk	jik
w/o optimization	2.1	2.1	2.9	2.9	2.9	2.9
with optimization	5.8	5.4	27	25	62	62
BLAS 3	100					

The big differences in performance are mainly due to memory access and cache optimization. The last line, with another improvement of a factor 1.5 compared to the best possible achieved so far, gives the Basic Linear Algebra Subroutines (BLAS) performance. This library is available for almost every computer today. The ingenious idea of BLAS was that only the function headers are specified, whereas the implementation for each individual computer is performed by the manufacturer.

The numbers presented show that we must be very much interested in using high-level routines and, whereever possible, in using BLAS.

3. Interval arithmetic. The product of two point matrices is easy to implement using BLAS. Suppose there is a routine `setround(m)` with the property that after the call `setround(-1)` the rounding mode is permanently switched downwards, i.e. every following operation is performed with rounding downwards according to the IEEE 754 standard [4] until the next call of `setround`. Accordingly, `setround(m)` shall switch the rounding to upwards for m=1, and to nearest for m=0.

Then the product of two point matrices $A \in M_{n,k}(\mathbb{F}), B \in M_{k,m}(\mathbb{F})$, $\mathbb{F}$ denoting the set of double precision floating point numbers, can be realized as follows.

```
setround(-1)
C.inf = A*B;
setround(1)
C.sup = A*B;
setround(0)
```

It follows

```
C.inf <= A*B <= C.sup
```

for comparison in a componentwise sense. Note that the proof is a successive use of the fact that, in case rounding is switched downwards, the sum and the product of two floating point numbers yields a floating point result definitely being less than or equal to the correct (real) result, whereas the floating point result is definitely greater than or equal to the exact result for rounding switched to upwards.

Note that this approach does not necessarily work for other composed operations. For example, it is not correct for triple matrix products. Similarly, the product of a point matrix $A \in M_{n,k}(\mathbb{F})$ and an interval matrix $\mathbf{B} \in \mathbb{I}M_{k,m}(\mathbb{F})$ cannot be computed by `A*B.inf` and `A*B.sup`. In [11] a method was proposed for fast computation of $A * \mathbf{B}$ using BLAS. The idea is the intermediate use of midpoint-radius representation.

```
setround(1)
Bmid = B.inf + 0.5*(B.sup-B.inf);
Brad = Bmid - B.inf;
setround(-1)
C1 = A * Bmid;
setround(1)
C2 = A * Bmid;
Cmid = C1 + 0.5*(C2-C1);
Crad = ( Cmid - C1 ) + abs(A) * Brad;
setround(-1)
C.inf = Cmid - Crad;
setround(1)
C.sup = Cmid + Crad;
```

ALGORITHM 3.1. *Point matrix times interval matrix*

The first three lines calculate a matrix pair `<Bmid,Brad>` with the property

$$\forall B \in \mathbf{B} : \texttt{Bmid} - \texttt{Brad} \leq B \leq \texttt{Bmid} + \texttt{Brad}$$

for the comparision in the componentwise sense. The next statements first compute an inclusion [C1,C2] of `A*Bmid`, and then take care of the radius `Brad`. The number of operations adds to $3n^3$ additions and $3n^3$ multiplications. This is 1.5 times more operations than necessary by the traditional implementation because the product of a floating point number and an interval can be performed with two multiplications (and a case distinction), and the interval addition requires two additions anyway. However, the following timings will demonstrate the vast improvement in performance of the new approach.

The only attempt to improve on the traditional implementation of interval matrix operations was the BIAS approach [5]. The following table gives the performance in "Miops" for multiplication of an nxn point times an nxn interval matrix for the traditional approach, for the BIAS approach and the above Algorithm 3.1. Timing is on a Convex SPP 200. Here the the matrix multiplication is counted as $2n^3$ interval operations, and a Miop are 1 Million interval operations.

Performance [Miops]	n=100	n=200	n=500	n=1000
traditional	6.4	6.4	3.5	3.5
BIAS	51	49	19	19
Algorithm 3.1	95	219	142	162

TABLE 3.2. *Performance for point matrix times interval matrix*

Obviously there is an immense improvement of performance by the new approach using BLAS routines. The decrease of performance of the BIAS library is due to cache misses. It could be improved by implementation of blocked algorithms. Note that the new Algorithm 3.1 uses BLAS, and therefore it uses blocked algorithms without effort on the part of the user. The varying performance of the new Algorithm 3.1 for different dimensions is also due to favourable and less favourable block sizes.

Another advantage of Algorithm 3.1 is that parallelization comes free of work. Just linking the parallel BLAS does the job. The BIAS approach can be parallelized as well, however, this has to be done by the user. The Convex SPP 200 allows us to use 4 processors, and performance data is as follows (for the traditional approach and the BIAS approach performance does not change unless special algorithms would be implemented).

Performance [Miops]	n=100	n=200	n=500	n=1000
Algorithm 3.1	142	551	397	526

TABLE 3.3. *Parallel performance for point matrix times interval matrix*

The gain in performance is not too from the magic factor 4. Note that this was achieved by merely linking the parallel BLAS library.

For the product of two interval matrices we also use an intermediate midpoint-radius representation. The performance number are even more impressing than before. However, there is a drawback to this, namely, that midpoint-radius product causes an overestimation of the true result whereas the infimum-supremum representation yields the sharp inclusion of the product of two interval matrices.

This would be a showstopper if overestimation would be arbitrarily severe. However, it can be shown that overestimation is globally bounded by a constant [11], and it is small if the input intervals are small. More precisely, define the relative precision $\mathrm{prec}(\mathbf{A})$ of an interval $\mathbf{A}$ by

$$\mathrm{prec}(\mathbf{A}) := \min\left(\frac{\mathrm{rad}(\mathbf{A})}{\mathrm{mid}(\mathbf{A})}, 1\right).$$

Let interval matrices $\mathbf{A}$ and $\mathbf{B}$ be given such that $\mathrm{prec}(\mathbf{A}_{ij}) \le e$ and $\mathrm{prec}(\mathbf{B}_{ij}) \le f$ for all i, j. Let $\mathbf{C}$ denote the result obtained by midpoint-radius arithmetic, and $\mathbf{A} * \mathbf{B}$ denote the true (and therefore narrowest) interval matrix product. Then the overestimation by midpoint-radius arithmetic satisfies

$$\frac{\mathrm{rad}(\mathbf{C})_{ij}}{\mathrm{rad}(\mathbf{A} * \mathbf{B})_{ij}} \le 1 + \frac{e \cdot f}{e + f} \le 1.5.$$

for all indices i, j. For example, input intervals with relative precision 1% suffer an overstimation of not more than 0.5% in radius.

If this small overestimation is critical, the traditional interval matrix multiplication or some variant [11] must be used. Otherwise the following performance data apply. Again, matrix multiplication is counted as $2n^3$ interval operations.

Performance [Miops]	n=100	n=200	n=500	n=1000
traditional	4.7	4.6	2.8	2.8
BIAS	4.6	4.5	2.9	2.8
Algorithm 3.1	9.1	94	76	99
Algorithm 3.1 parallel	9.5	145	269	334

TABLE 3.4. *Performance for interval matrix times interval matrix*

Implementation of complex vector and matrix operations is easily done by computing real and imaginary part. The implementation in Matlab is straightforward because all vector and matrix operations are already available. Thus the new approach also solves the problem of interpretation overhead.

Moreover, the above approach also applies to sparse matrices. As sparse matrices are already an intrinsic data type in Matlab, an implementation comes without any additional work.

A first simple application example is the check of nonsingularity of a given interval matrix $\mathbf{A} \in \mathbb{I}M_n(\mathbb{F})$. A well-known sufficient criterion for $\mathbf{A} \in \mathbb{I}M_n(\mathbb{F})$ being nonsingular is that for some matrix R and some interval vector $\mathbf{X}$

$$(I - R\mathbf{A}) \cdot \mathbf{X} \subseteq \mathrm{int}(\mathbf{X}),$$

is satisfied. A simple implementation of this criterion is

```
R = inv(A.mid);
C = eye(n) - R*A;
X = infsup(-1,1)*ones(n,1);
Y = C*X;
res = all( ( X.inf<Y.inf ) & ( Y.sup<X.sup ) );
```

If `res`=1 after execution, every real matrix enclosed in the interval matrix $\mathbf{A}$ is proved to be nonsingular. The above is only an example for ease of use.

4. Nonlinear problems. For application of verification methods to nonlinear problems especially the inclusion of derivatives of functions over a range is needed as well as interval elementary functions. Gradients can be computed using an operator concept and automatic differentiation [8]. The implementation is simplified by the vector and matrix operations in Matlab.

Automatic differentiation is one way to obtain an expansion of a certain function. Another method to obtain such information are slopes, where the function is expanded with respect to a point or an interval. Standard slopes are defined in [7]; an extension, which is used in Matlab, has been developed in [9] and used in [3]. Corresponding toolboxes for gradients and slopes are included in INTLAB.

When defining a function, a user friendly way would use the same source code for evaluation of the function at some real or complex floating point number, for the evaluation of the range of the function, for gradient information or for the gradient of the function over a certain range. This causes a specific problem. Consider the sample function

$$f(x) = \sin(\pi x).$$

A Matlab implementation is

```
function y = f(x)
  y = sin(pi*x);
```

There are no problems when inserting a (real or complex) floating point number `x`, a gradient value or a slope value. Problems occur when inserting an interval `X`. In this case the user may want to use an inclusion of the irrational number π in the definition of the function. Otherwise a call `y = f(intval(1))` may produce an interval not containing zero because the floating point approximation `pi` of π is used instead. A redefinition

```
function y = f(x)
  Pi = midrad(pi,1e-16);
  y = sin(Pi*x);
```

would calculate a correct inclusion `Pi` for π and deliver a correct inclusion for zero when calling `f(intval(1))`. However, the simple call `f(1)` would yield an unexpected interval answer. Obviously, the type of the result shall depend on the type of the input argument `x`: For interval input the computation should be performed in interval arithmetic with correct interval data for π, for floating point input the Matlab internal approximation `pi` is sufficient and a floating point approximate result should be delivered.

The solution to the dilemma are two functions to adjust the type of a constant. Consider

```
function y = f(x)
  Pi = typeadj( midrad(pi,1e-16) , typeof(x) );
  y = sin(Pi*x);
```

In this implementation `typeof(x)` returns type information about the input parameter x. Especially, this is "intval" for interval input and "double" for floating point input. The statement `typeadj(a,type)` adjusts the type of the input `a` to the type `type`. Especially, in case `type` is "double", the midpoint of `a` is returned. This allows to write one source code for various applications, from pure floating point computation to complex interval gradients and others.

The above implementation requires rigorous standard functions. This has been indeed a major task in previous approaches. Following we present a very simple method to implement rigorous standard functions over real and complex intervals.

5. Standard functions. For single precision it is in principle possible to test all values of a built-in standard function for their accuracy and to add a suitable error margin. For double precision this is not possible.

Usually the built-in standard functions are very accurate, and it is seldom that a value is not correctly rounded to least significant bit accuracy. In fact, we rarely found cases where the computed result is off by more than one bit - at least for arguments in a reasonable range. However, there is no proof for the accuracy of the results, and in order to achieve truely rigorous results a guess of accuracy is not sufficient.

The idea is to use a table approach together with some correction formulas. Take, for example, the exponential. We suppose that multiple precision functions $\underline{F}, \overline{F}$ are available such that for a given floating point number $x \in \mathbb{F}$ it is

$$\underline{F}(x) \le e^x \le \overline{F}(x)$$

with high accuracy. Define

$$R_{\exp} := \{\pm(0, 1, \ldots, 2^{14} - 1) \cdot 2^{-14}\} \subseteq \mathbb{F}$$

as a reference set for the exponential. For given $x \in \mathbb{F}$ define $y = \exp_\square(x) \in \mathbb{F}$ to be the floating approximation computed by the given (floating point) exponential function. Then the error of such approximations over the reference set is defined as follows.

$$\begin{aligned} \underline{\varepsilon} &:= \max_{\substack{x \in R_{\exp} \\ y = \exp_\square(x)}} \{(y - \underline{F}(x))/|y|\}, \\ \overline{\varepsilon} &:= \max_{\substack{x \in R_{\exp} \\ y = \exp_\square(x)}} \{(\overline{F}(x) - y)/|y|\}. \end{aligned}$$

A short computation yields

$$y - \underline{\varepsilon} \cdot |y| \le e^x \le y + \overline{\varepsilon} \cdot |y|.$$

Now lower and upper bounds for the left hand side and right hand side, respectively, are computable for every $x \in R_{\exp}$ by

```
ys = exp(x);
setround(-1)
y.inf = ys + (-eps)*abs(ys);
setround(1)
y.sup = ys + eps*abs(ys);
```

with the property

$$\texttt{y.inf} \le e^x \le \texttt{y.sup} \quad \forall x \in R_{\exp}$$

where eps:$= \varepsilon_{\exp}$. The point is that $\underline{F}(x), \overline{F}(x)$ for all $x \in \mathbb{IR}_{\exp}$ and $\varepsilon_{\exp}$ have to be computed *only once*. From then on the constant $\varepsilon_{\exp}$ is a system constant to be used in the further computations. For arbitrary $X \in \mathbb{IF}$ inclusions of the exponential are computed as follows. In an initialization procedure we compute floating point numbers $E_\nu, \underline{E}_\nu, \overline{E}_\nu$ with

$$E_\nu + \underline{E}_\nu \le e^\nu \le E_\nu + \overline{E}_\nu \quad \text{for } -744 \le \nu \le 709.$$

For $x \le -745$ or $x \ge 710$, e^x is outside the double precision floating point range. For $X \in \mathbb{IF}$, split $X := X_{\text{int}} + x$ with $X_{\text{int}} = \text{sign}(X) \cdot \lfloor |X| \rfloor \in R$ and $-1 < x < 1$. Furthermore, set

$$\begin{aligned} \widetilde{x} &= 2^{-14} \cdot \lfloor 2^{14} x \rfloor \\ d &= x - \widetilde{x}. \end{aligned}$$

Then $\widetilde{x}$ has no more than 14 leading bits in its binary representation and $\widetilde{x} \in R_{\exp}$. This implies

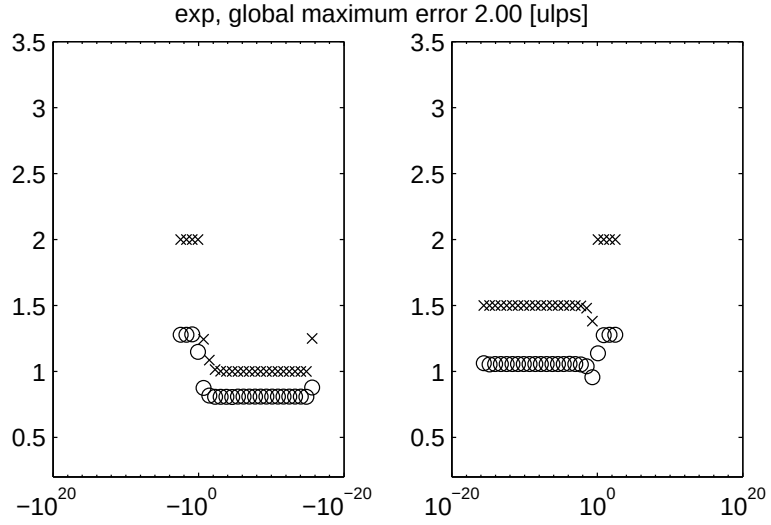
$$e^x = e^{\widetilde{x}} \cdot e^d \quad \text{with} \quad \sum_{i=0}^{3} \frac{d^i}{i!} \le e^d \le \sum_{i=0}^{3} \frac{d^i}{i!} + e \cdot \frac{d^4}{4!}.$$

By the choice of the reference set it is $0 \le d < 2^{-14}$ and

$$e \cdot \frac{d^4}{4!} \le 0.68d \cdot \frac{d^3}{3!} < 1.6 \cdot 10^{-18}.$$

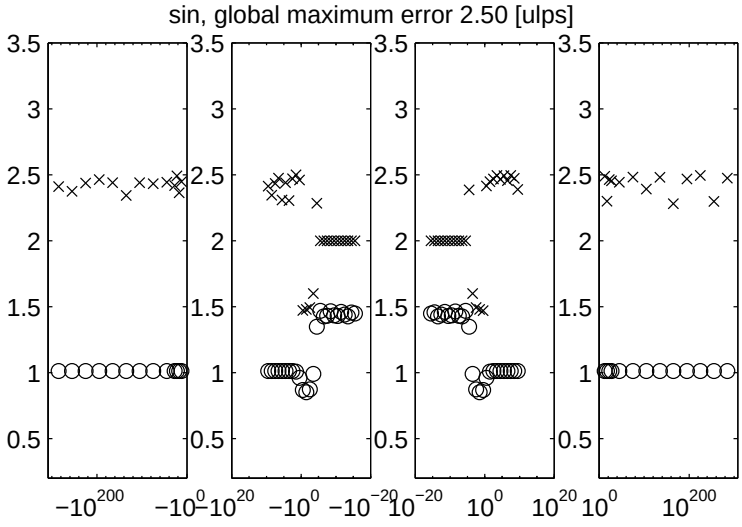
Putting things together yields rigorous bounds for the value of the exponential over the entire floating point range.

Corresponding reference sets and formulas for splitting arguments have been developed for all elementary standard functions. A careful implementation of the formulas yields standard functions of very high accuracy, in fact always better than 3 ulp. For example, the relative error for the exponential, tested over some 50 Million test cases, looks as follows. Here crosses depict the maximum relative error of the lower and upper bounds against each other over a certain domain, whereas the circles depict the average error.



GRAPH 5.1. *Accuracy exponential*

The maximum error is not more than 2 ulps, whereas the average relative error is about 1 ulp. Even for the trigonometric functions, where problems with argument reduction may cause significant cancellation errors, high accuracy is achieved. For example, the error plot for the sine is as follows.



GRAPH 5.2. *Accuracy sine*

The test set for the sine comprises of some 100 Million floating point numbers in the range from -10^{300} to 10^{300}.

Guaranteed accuracy does not come free of cost, expecially when the entire implementation is performed in Matlab itself, suffering from interpretation overhead. For the sine of a single floating point number the verified computation takes about 700 times the computing of an approximate computation. However, the first is correct to the last digit, whereas, especially for large arguments, the latter may be afflicted with large errors. For example,

```
format long; x = 2^60; sin(x), sin(intval(x))
```

produces the answer

```
x =
    1.152921504606847e+018
ans =
  -0.83147474810936
intval ans =
  -0.83064921763725
```

where only the first two digits of the floating point approximation are correct. For vector input interpretation overhead decreases. For example, vectors of length 100 take about 200 times more computing for the verified sine.

The computing time for trigonometric functions suffers from argument reduction. In a C- or Fortran imlementation the factor would be much smaller. Other functions behave much better. In the following table we list timings for exp and atan on a 300 MHz Pentium I Laptop for input vector x with n components.

time	n=1	n=100
[msec]	approx./verified/factor	approx./verified/factor
exp	0.03 / 3.9 / 152	0.22 / 7.7 / 35
atan	0.02 / 3.5 / 164	0.10 / 6.4 / 58

From the times it can also be seen that computing time for verified computation only doubles when going from one double number to a vector with 100 components. This is mainly due to interpretation overhead.

For the other standard functions similar considerations are possible. The formulas must be developed carefully in order to maintain the anticipated accuracy of 3 ulp. This has been performed for exp, log, log10, the trigonometric functions and their inverse functions, and for the hyperbolic functions and their inverses. All are included in the new version INTLAB.

For complex interval functions we use the results obtained by Börsken [2]. Denote for given $a \in \mathbf{C}, 0 \le r \in \mathbb{IR}$

$$A =< a, r >:= \{z \in \mathbf{C} : |z - a| \le r\}.$$

Then Börsken defines the midpoint of $f(A)$ to be $f(a)$ and shows

$$\begin{array}{lcl} \exp(< a, r >) & \subseteq & < \exp(a), |\exp(a)| \cdot (\exp(r) - 1) > \\ \log(< a, r >) & \subseteq & < \log(a), -\log(1 - r/|a|) > \\ \mathrm{sqrt}(< a, r >) & \subseteq & < \mathrm{sqrt}(a), |\sqrt{|a| - r} - \sqrt{|a|}| > . \end{array}$$

These bounds are sharp for certain arguments. However, in other cases there may be quite some overestimation due to the choice of the midpoint. However, other formulas defining a different and more optimized midpoint with respect to, for example, the area of the inclusion may become quite involved. To our knowledge nothing is known in this direction, a research opportunity.

Having those three standard function all other mentioned standard functions can be expressed by those using standard formulas. Doing this another problem occurs. Complex standard functions are usually defined by some main value. This causes discontinuities. For example, $\sqrt{-4} = +2i$, but $\sqrt{-4 + \varepsilon i}$ for small $\varepsilon < 0$ yields a value near $-2i$. This causes problems when an interval approaches the negative real axis and if $f(X)$ for a complex interval X is defined to enclose the result of the usual power set operation

$$f(\mathbf{X}) := \{f(x) : x \in \mathbf{X}\}.$$

We choose for the moment to use the above formulas. This implies that for a given function f the following weaker statement is true:

$$\mathbf{Y} = f(x) \Rightarrow \forall x \in \mathbf{X} \exists y \in \mathbf{Y} : f^{-1}(y) = x.$$

There is also space for future development and research.

6. Long arithmetic. Finally, the above approach for the definition of standard functions requires some multiple precision arithmetic with error bounds. There are a number of such packages available, for example [1] only to mention one. However, we choose to write a package in Matlab in order to maintain best possible portability.

The data type *long* has the structure

```
C.sign       in {-1,1}
C.mantissa   in 0 .. beta-1
C.exponent   representable integer ( -2^52+1 .. 2^52-1 )
C.error      nonnegative double, stored by C.error.mant and C.error.exp
```

representing the long number

$$\texttt{C.sign} \cdot \sum_{\nu=1}^{n} \texttt{C.mantissa}_\nu \cdot \beta^{\texttt{C.exponent}-\nu},$$

where `C.mantissa` is an array of length n corresponding to the precision in use. The field `C.error` is optional; if specified it represents the number

$$\texttt{C.error.mant} \cdot \beta^{\texttt{C.error.exp}},$$

where both `C.error.mant` and `C.error.exp` are nonnegative double numbers. It is interpreted as the radius of an interval with the above midpoint. Therefore the radius is stored in only two double numbers, whereas the midpoint is stored in an array of double numbers. The basis β is a system constant. It is a power of 2; usually 2^{25} is used.

The definition of multiple precision arithmetic is standard. For the current implementation we have two additional difficulties. First, it is no integer arithmetic but a long floating point arithmetic (to base beta). This makes addition and subtraction more involved. Secondly, all long routines are written to support vector input in a vectorized computation. Treating vectors one component after the other causes a significant interpretation overhead. For example, given two long vectors X and Y of length 100 and precision of 500 decimal places, calculation of the 100 products $X(i) * Y(i)$ by

```
for i=1:100, Z(i) = X(i)*Y(i); end
```

takes 25.9 sec, whereas the vectorized multiplication

```
Z = X.*Y;
```

takes only 0.6 sec on a 300 MHz Pentium I Laptop. Otherwise, the vectorized operations in Matlab can be used. For example, the multiplication of multiple precision numbers is a convolution and already built into Matlab.

7. An example of INTLAB code. Finally we give an example of INTLAB code to demonstrate its ease of use and readability. We print the full code to compute inclusions of multiple eigenvalues and corresponding invariant subspaces for a given (real or complex, not necessarily symmetric or Hermitian) matrix. We also give the full code how to call the algorithm. So the following is executable code in INTLAB under Matlab.

```
function [L,X] = VerifyEig(A,lambda,xs)
%VERIFYEIG      Verification of eigencluster near (lamda,xs)
%
%   [L,X] = VerifyEig(A,lambda,xs)
%
%For an eigenvalue cluster near lambda, where xs(:,i), i=1:k is an
%  approximation to the corresponding invariant subspace
%
%On output, L contains (at least) k eigenvalues of A, and X
%  includes a base for the corresonding invariant subspace
%By principle, L is a complex interval
%

% written  07/15/99     S.M. Rump
%

  [n k] = size(xs);

  [N,I] = sort(sum(abs(xs),2));
  u = I(1:n-k);
  v = I(n-k+1:n);
  midA = mid(A);

  % one floating point iteration
  R = midA - lambda*speye(n);
```

```
R(:,v) = -xs;
y = R\(midA*xs-lambda*xs);
xs(u,:) = xs(u,:) - y(u,:);
lambda = lambda - sum(diag(y(v,:)))/k;

R = midA - lambda*speye(n);
R(:,v) = -xs;
R = inv( R );
C = A - intval(lambda)*speye(n);
Z = - R * ( C * xs );
C(:,v) = -xs;
C = speye(n) - R * C;
Y = Z;
Eps = 0.1*abs(Y)*hull(-1,1) + midrad(0,realmin);
m = 0;
mmax = 15 * ( sum(sum(abs(Z(v,:))>.1)) + 1 );
ready = 0;
while ( ~ready ) & ( m<mmax ) & ( ~any(isnan(Y(:))) )
  m = m+1;
  X = Y + Eps;
  XX = X;
  XX(v,:) = 0;
  Y = Z + C*X + R*(XX*X(v,:));
  ready = all(all(in0(Y,X)));
end

if ready
  M = abs(Y(v,:));                          % eigenvalue correction
  [Evec,Eval] = eig(M);
  [rho,index] = max(abs(diag(Eval)));
  Perronx = abs(Evec(:,index));
  setround(1);
  rad = max( ( M*Perronx ) ./ Perronx );    % upper bound for Perron root
  setround(0)
  L = tocmplx(midrad(lambda,rad));
  Y(v,:) = 0;
  X = xs + Y;
else
  disp('no inclusion achieved')
  X = NaN*ones(size(xs));
  L = NaN;
end
```

ALGORITHM 7.1. *Rigorous inclusion of multiple eigenvalues*

The algorithms follows [10] to be published in Linear Algebra and it Applications. It is based on the following.

For $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ denote by $A \in M_n(\mathbb{K})$ an $n \times n$ matrix, by $\widetilde{X} \in M_{n,k}(\mathbb{K})$ an approximation to an invariant subspace corresponding to a multiple or a cluster of eigenvalues near $\widetilde{\lambda} \in \mathbb{K}$, such that $A\widetilde{X} \approx \widetilde{\lambda}\widetilde{X}$.

The degree of arbitrariness is removed by freezing k rows of the approximation $\widetilde{X}$. If the set of the remaining rows is denoted by u, then we denote by $U \in M_{n,n-k}(\mathbb{R})$ the submatrix of the identity matrix with columns

in u. Correspondingly, we set $v := \{1,\ldots,n\}\backslash u$ and define $V \in M_{n,k}(\mathbb{R})$ to comprise of the columns in v out of the identity matrix. That means $UU^T + VV^T = I$, and $V^T\widetilde{X}$ is the normalizing part of $\widetilde{X}$. Then the following is true [10].

THEOREM 7.2. *Let $A \in M_n(\mathbb{K}), \widetilde{X} \in M_{n,k}(\mathbb{K}), \widetilde{\lambda} \in \mathbb{K}, R \in M_n(\mathbb{K})$ and $\mathbf{X} \in \mathbb{I}M_{n,k}(\mathbb{K})$ be given, and let U, V partition the identity matrix as defined before. Define*

$$f(\mathbf{X}) := -R(A\widetilde{X} - \widetilde{\lambda}\widetilde{X}) + \{I - R\big((A - \widetilde{\lambda}I)UU^T - (\widetilde{X} + UU^T \cdot \mathbf{X})V^T\big)\} \cdot \mathbf{X}.$$

Suppose

$$f(\mathbf{X}) \subseteq \mathit{int}(\mathbf{X}).$$

Then there exists $\widehat{M} \in M_k(\mathbb{K})$ with $\widehat{M} \in \widetilde{\lambda}I_k + V^T\mathbf{X}$ such that the Jordan canonical form of $\widehat{M}$ is identical to a $k \times k$ principal submatrix of the Jordan canonical form of A, and there exists $\widehat{Y} \in M_{n,k}(\mathbb{K})$ with $\widehat{Y} \in \widetilde{X} + UU^T\mathbf{X}$ such that $\widehat{Y}$ spans the corresponding invariant subspace of A.

Following we give two examples how to call the algorithm. The first one generates a random matrix, calculates approximations for the eigenvalues and eigenvectors and calls the algorithm for the first approximate eigenvalue/eigenvector pair. Note that `[V,D] = eig(A)` calculates a matrix `V` of eigenvectors and diagonal matrix `D` of eigenvalues such `A*X` is approximately equal to `X*D`. Furthermore, `rand` produces random numbers uniformly distributed in the interval [0,1] such that the entries of `A` are uniformly distributed within [-1,1].

```
n = 100; A = 2*rand(n)-1;
tic, [V,D] = eig(A); toc
tic, [L,X] = VerifyEig(A,D(1,1),V(:,1)); toc
format long
L
```

This produces the following output:

```
elapsed_time =
   0.6100
elapsed_time =
   0.9900
intval L =
  -4.6875246581698_ +  3.4404126988075_i
```

The underscore in the output of the inclusion `L` of the eigenvalue indicates that the last digit of the real and the imaginary part is uncertain. More precisely, subtracting and adding one to the last displayed figure (before the underscore) yields a correct inclusion. Note that input/output is also rigorous by means of specific INTLAB routines for interval I/O [12].

The second example produces a triple eigenvalue 1 together with some randomly choosen 97 eigenvalues, and eigenvector space in $[-1, 1]$.

```
X = 2*rand(100)-1; A = X * diag([1 1 1 2*rand(1,97)-1]) * inv(X);
tic, [V,D] = eig(A); toc
index = find( abs(diag(D)-1)<1e-12 );
k = index(1);
tic, [L,X] = VerifyEig(A,D(k,k),V(:,index)); toc
format long
L
```

The result is as follows.

```
elapsed_time =
   0.5000
elapsed_time =
   0.9900
intval L =
   1.000000000000__ -  0.000000000000__i
```

There are many more examples including ill-conditioned ones in the paper cited above [10]. Here our main objective is ease of use and readability. Note especially the index notation in Algorithm 7.1.

8. Conclusion. We presented some of the main ideas of the toolbox INTLAB for Matlab. INTLAB is available in its third release for PCs, a number of workstations and mainframes. More details can be found in [12]. The only machine dependency is the routine `setround` for switching the rounding mode. This assembly language routine is available for a number of machines. In Release 5.3 of Matlab under Windows even this is a built-in routine of Matlab. Then the entire toolbox is plain Matlab code.

All other code, some 362 functions and some 20 kLOC, is written in Matlab and therefore as portable as it can be. INTLAB is freely available for non-profit use from our homepage.

REFERENCES

[1] O. Aberth and M. Schaefer. C++ Module for Range Arithmetic, August 1991.

[2] N.C. Börsken. Komplexe Kreis-Standardfunktionen (Diplomarbeit). Freiburger Intervall-Ber. 78/2, Inst. f. Angewandte Mathematik, Universität Freiburg, 1978.

[3] J.B.S. de Oliveira. *Slope methods for sharper interval inclusions and their application to global optimization.* Dissertation, TU Hamburg-Harburg, 1996.

[4] *ANSI/IEEE 754-1985, Standard for Binary Floating-Point Arithmetic*, 1985.

[5] O. Knüppel. PROFIL / BIAS — A Fast Interval Library. *Computing*, 53:277–287, 1994.

[6] MATLAB User's Guide, Version 5. The MathWorks Inc., 1997.

[7] A. Neumaier. *Interval Methods for Systems of Equations.* Encyclopedia of Mathematics and its Applications. Cambridge University Press, 1990.

[8] L.B. Rall. Automatic Differentiation: Techniques and Applications. In *Lecture Notes in Computer Science 120.* Springer Verlag, Berlin-Heidelberg-New York, 1981.

[9] S.M. Rump. Expansion and Estimation of the Range of Nonlinear Functions. *Mathematics of Computation*, 65(216):1503–1512, 1996.

[10] S.M. Rump. Computational Error Bounds for Multiple or Nearly Multiple Eigenvalues. LAA, to appear, 1999.

[11] S.M. Rump. Fast and parallel interval arithmetic. *BIT*, 39(3):539–560, 1999.

[12] S.M. Rump. INTLAB - INTerval LABoratory. In Tibor Csendes, editor, *Developements in Reliable Computing*, pages 77–104. Kluwer Academic Publishers, 1999.