



SCIENTIFIC COMPUTING
SOFTWARE ENGINEERING
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**intpakX:
A Maple Power Tool for verified numerical computing**

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Overview

1. `intpakX` - History
2. `intpakX` - Functional Range and Realization
 - Real Interval Arithmetic
 - Complex Disc Arithmetic
3. `intpakX` - Applications and Examples
 - Interval Newton Method
 - Range Enclosure (2D and 3D)
 - Complex Disc Arithmetic
 - Validation of numerical output of existing programs
 - Multiple Precision Interval Arithmetic

History

- 1993: `intpak` by R. Corless and A. Connell
 - Interval Type
 - Basic Arithmetic operations
 - Standard Functions
- 1999: `intpakX` by W. Krämer and I. Geulig (Add-on)
 - Interval Newton Method
 - Range Enclosure
 - Complex Disc Arithmetic
 - Graphical output

intpakX V1.0

- New version (running from Maple 6 up)
- Integrates `intpak` and `intpakX` (formerly separate packages)
- Redesign as Maple-Module
- Language integration
- Bug Fixes
- Published as a *Maple PowerTool Interval Arithmetic* in 2002/2003

Real Intervals

Interval type:

- Maple **List** with additional properties
(i.e. intervals $[x_1, x_2]$,
 x_1, x_2 float or \pm infinity, $x_1 \leq x_2$)
- **construct**, **convert** and **inapply** („interval unapply“)

Operators and standard functions

- Operators $\&+$, $\&-$, $\&*$, $\&/$ for intervals
- Additional function for extended division
- interval intersection/union
- Power, square/root, logarithm and exponential functions
- trigonometric functions

→ Verified computations with guaranteed interval bounds possible.

Applicability

- suited for numerical computations using the operators described above or using the applications presented later

Effects to be paid attention to:

- Computations that need procedures other than the ones mentioned or that need to identify special operators; i.e. the `degree` function does not work with interval polynomials like

`[1.0,2.0] &* x^2 &+ [-1.5,-1.0]`

- No automatical simplification of functions:

`A &+ 2 &* A` is *not* simplified into `3 &* A.`
(can affect the success of symbolical computations).

Complex Intervals

- Disc intervals: `List` with three numerical values, interpreted as midpoint and radius (non-negative) of the disc
- Arithmetic operations: `&cadd`, `&csub`, `&cmult`, `&cdiv` (centered)
- Additional: Area-optimal multiplication and division
- Exponential function for complex discs

Applications (I) (real)

Interval Newton Method

Iteration:

$$[x]^0 := [x], \quad [x]^{k+1} := \left(m([x]^k) - \frac{f(m([x]^k))}{f'([x]^k)} \right) \cap [x]^k$$

$m([x]^k)$ midpoint of $[x]^k$

- Computes enclosing intervals for *all* zeros of a cont. diff. function f with guaranteed bounds
- arbitrary start interval
- automatical use of interval operators/functions
- adjustable precision (digits, diameter of solution interval) and number of iterations
- graphical output of iteration steps (optional)

Applications (II) (real)

Range Enclosure

- for real-valued functions of one or two real variables
- in 2D, interval evaluation and mean value form are combined
- in 3D, only interval evaluation is done
- iterative interval subdivision
- automatical use of interval operators/functions
- adjustable number of iterations

Applications (III) (complex)

Range Enclosure for Complex Polynomials

- Range Enclosure based on a Horner-Scheme using centered multiplication

`&horner_eval_cent`

- Range Enclosure based on a Horner-Scheme using area-optimal multiplication

`&horner_eval_opt`

- Range Enclosure using centered forms (similar to mean value form for real numbers)

`¢red_form_eval`

Example 1: Interval Newton Method

Enclosure of the zeros of

$$f := x - \sin(\exp(\sqrt{x-2}));$$

on the interval [8.,10.]:

Load `intpakX`:

```
> restart;
> libname:="/opt/lib/mymaplelib", libname;
> with(intpakX);
```

Enclose zeros:

```
> f:=x->sin(exp(sqrt(x-2)));
> X:=[8.,10.];
> compute_all_zeros_with_plot(f,X,0.001);
```

$$f := x \rightarrow \sin(\exp(\sqrt{x-2}))$$

```
> compute_all_zeros_with_plot(f,X,0.001,10,10);
```

Digits = 10

Iteration step 1

xold= [8., 10.]

xnew1= [9.289288473, 10.]

xnew2= [8., 8.710711527]

Iteration step 2

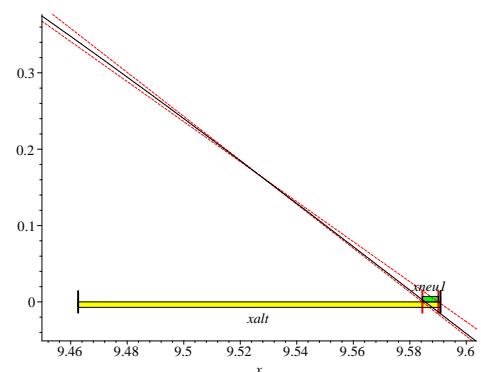
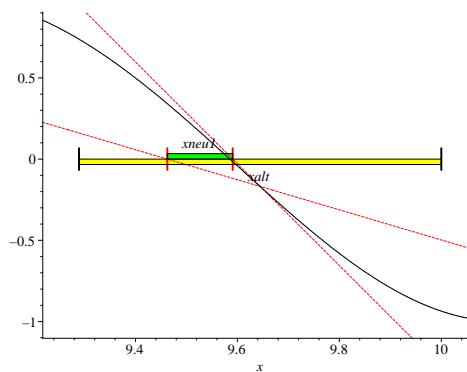
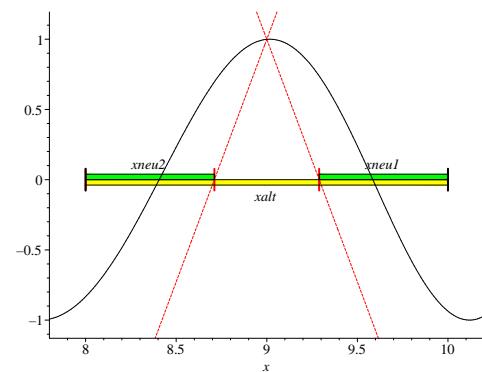
xold= [9.289288473, 10.]

xnew1= [9.462634907, 9.590834649]

Iteration step 3

xold= [9.462634907, 9.590834649]

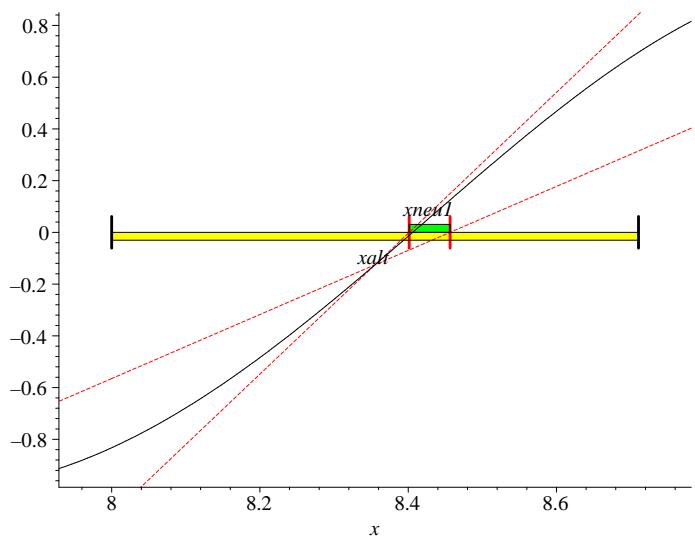
xnew1= [9.584440425, 9.590102305]



Iteration step 4

xold= [8., 8.710711527]

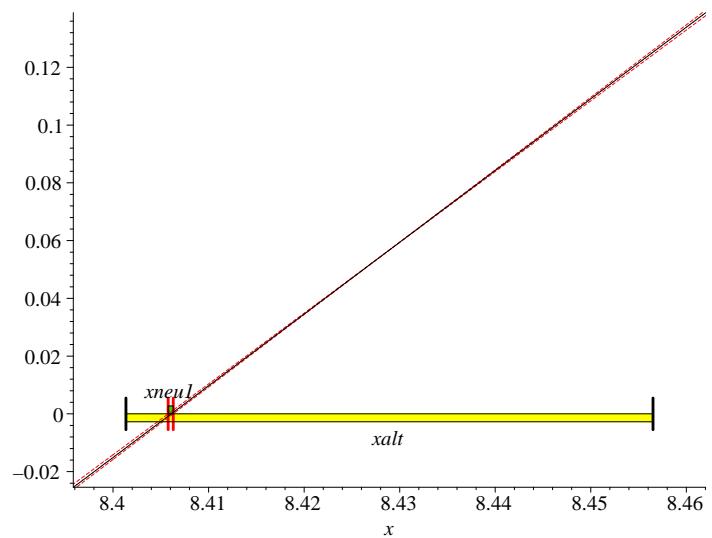
xnew1= [8.401353571, 8.456507702]



Iteration step 5

xold= [8.401353571, 8.456507702]

xnew1= [8.405771237, 8.406299401]



Example 2: Range Enclosure (2D)

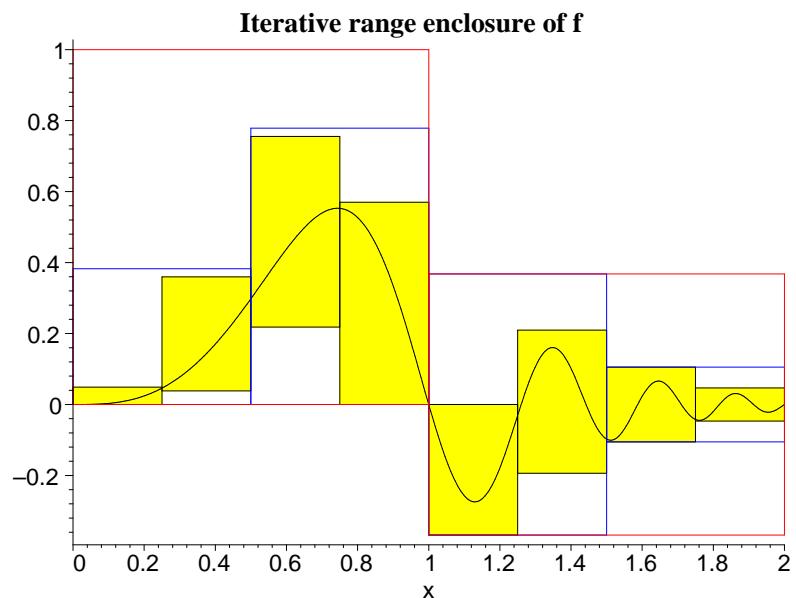
Range Enclosure of

```
f:=x->exp(-x^2)*sin(Pi*x^3);
```

```
> f:=x->exp(-x^2)*sin(Pi*x^3);
> X:=[0.,2.];
> compute_range(f,X,3);
```

Start range enclosure = [-1.000000002, 1.000000002]

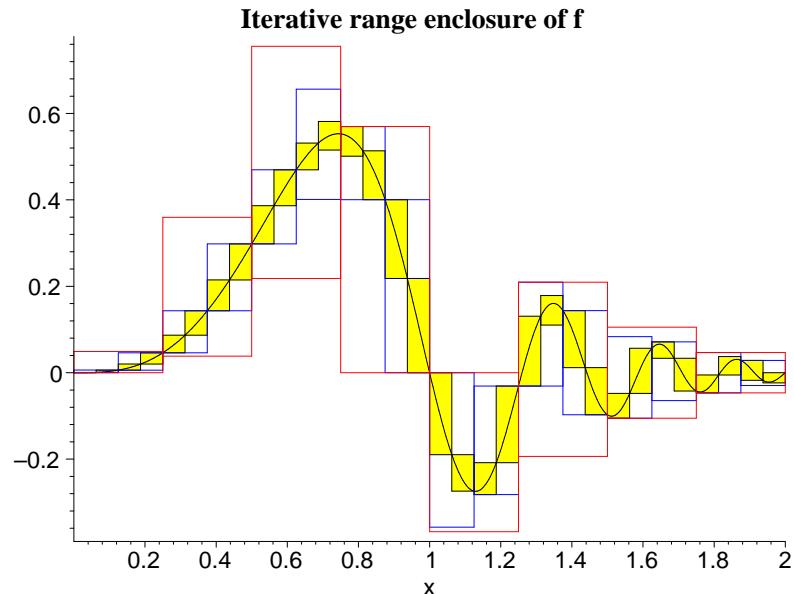
Range enclosure after step 3 = [-.3678794418,.7554611004]



```
> compute_range(f,X,5);
```

Start range enclosure = [-1.000000002, 1.000000002]

Range enclosure after step 5 = [-.2820629525,.5815483768]



Example 2: Range Enclosure (2D)

- Reasonable results displayed after few iteration steps
- Numerical values available in variables
`list_of_intervals` and `list_of_ranges`

```
> list_of_ranges;  
  
[[.2980341562, .3644580713], [.3644580699, .4296256944], [.4296256931, .4877217319],  
 [.4877217307, .5314384278], [.5314384254, .5523340343], [.5348860212, .5680755514],  
 [.4922683804, .5417224422], [.4003403046, .4922683817], [.2688894620, .4003403067],  
 [.1101516556, .2688894645], [-.5312103680e-1, .1101516586], [-.1896402434, -.5312103191e-1],  
 [-.2663280673, -.1896402391], [-.2920842800, -.2460035260], [-.2599399733, -.1706423650],  
 [-.1706423681, -.3075637699e-1], [-.3075637973e-1, .1002647343], [.1002647315, .1599864556],  
 [.1197822643, .1643652721], [.1173607362e-1, .1197822664], [-.8297860010e-1, .1173607573e-1],  
 [-.1104304755, -.7204027092e-1], [-.9203610994e-1, -.1800481925e-1],  
 [-.1800482181e-1, .5649041403e-1], [.4840145700e-1, .7131668286e-1],  
 [-.1254422882e-1, .5228321860e-1], [-.5212547117e-1, -.1065394717e-1],  
 [-.4426684404e-1, -.5350768968e-2], [-.5350770488e-2, .3072094080e-1],  
 [.6012399421e-2, .3151551268e-1], [-.2177923802e-1, .6012400536e-2],  
 [-.2204438709e-1, .4408877421e-9]]
```

Example 3: Range Enclosure (3D)

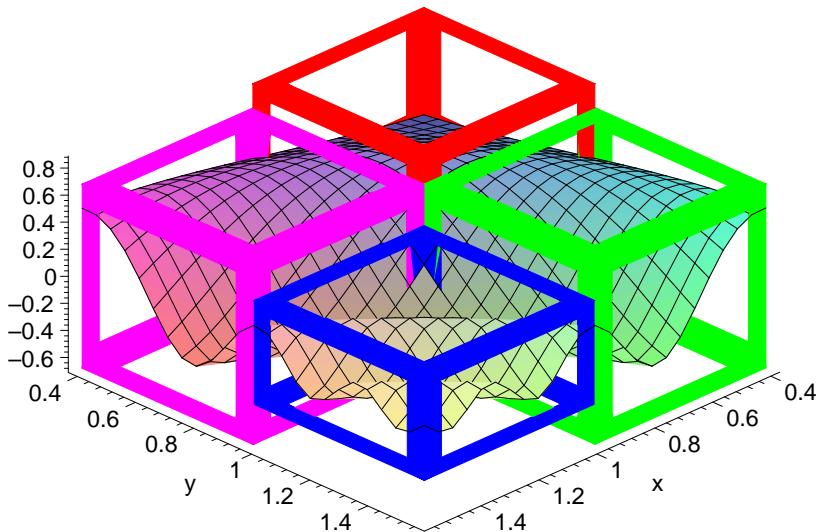
```
g:=(x,y)->exp(-x*y)*sin(Pi*x^2*y^2);
```

Evaluation on the interval

$[\frac{\pi}{8}, \frac{\pi}{2}] \times [\frac{\pi}{8}, \frac{\pi}{2}]$:

```
> compute_range3d(g,T,S,2);
```

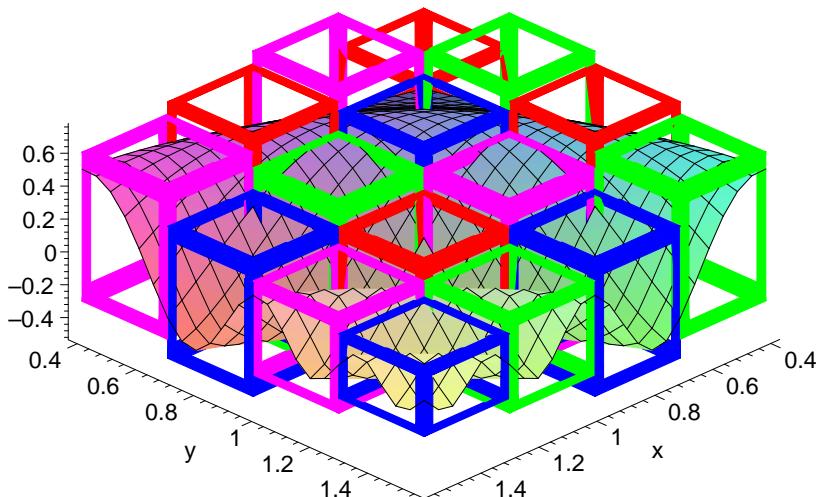
```
Start range enclosure = [-.8570898115, .8570898115]  
Range enclosure after step 1 = [-.8570898115, .8570898115]  
Range enclosure after step 2 = [-.6800891261, .8570898115]
```



$$g := (x, y) \rightarrow \exp(-x * y) * \sin(\pi * x^2 * y^2);$$

```
> compute_range3d(g,T,S,4);
```

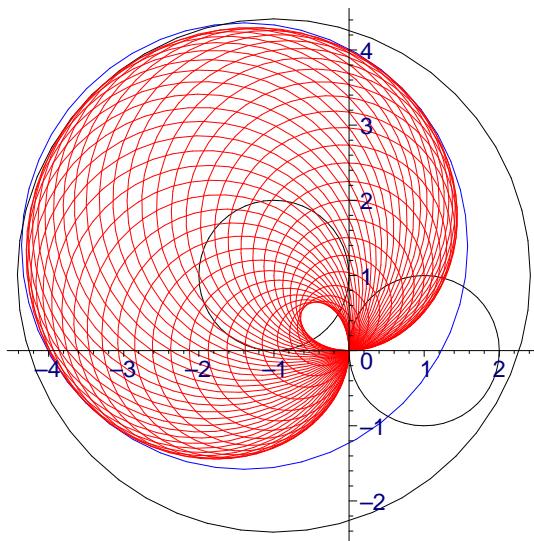
Start range enclosure = ', [-.8570898115, .8570898115]
Range enclosure after step 1 = [-.8570898115,.8570898115]
Range enclosure after step 2 = [-.6800891261,.8570898115]
Range enclosure after step 3 = [-.6800891261,.8486122905]
Range enclosure after step 4 = [-.5093193828,.7559256232]



Example 4: Complex Arithmetic

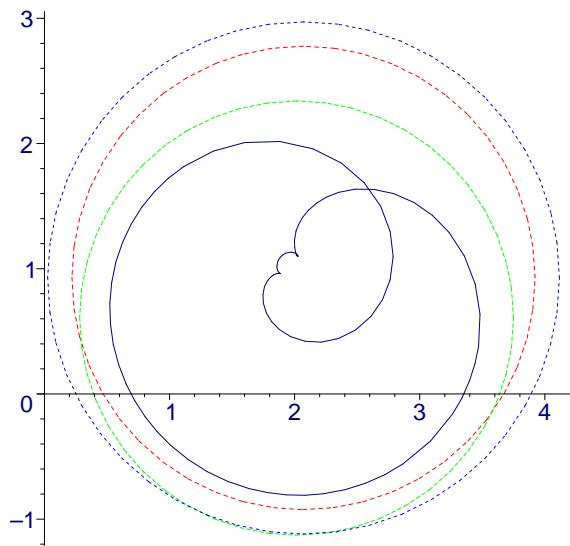
Multiplication of $\langle 1, 1 \rangle$ and $\langle -1+i, 1 \rangle$

- with centered multiplication
- with area-optimal multiplication



Ex.5: Range Enclosure (Complex Polynomials)

$$p := (0.1 + 0.1i)z^5 + 0.2iz^4 - 0.1iz^3 + (-0.2 - 0.1i)z + 2.0 + 1.0i;$$



Results using Horner-Scheme with centered and area-optimal multiplication and centered form.

Further Applications

Validation of numerical output

- **Objective:** Check results of an existing program
(here: integral equation solver)
- Result given as Taylor coefficients → Taylor expansion of exact result with verified coefficient enclosures needed

Example (Kress):

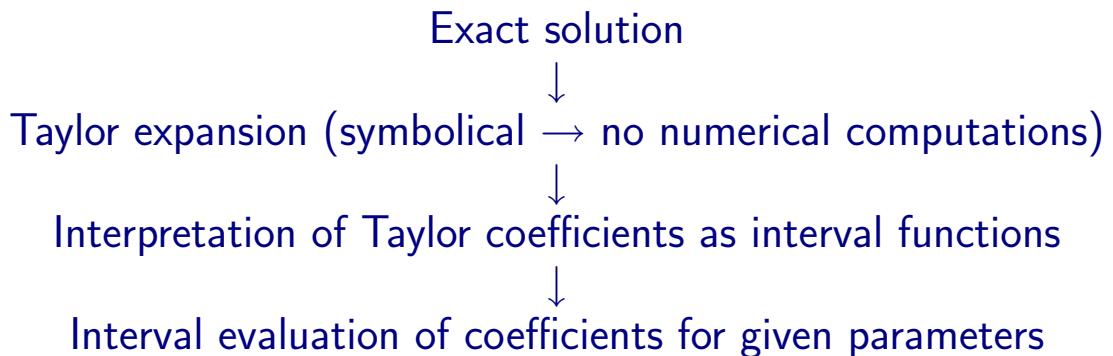
$$k(s, t) = (s + 1) \cdot e^{-st}$$
$$g(s) = e^{-s} - \frac{1}{2} + \frac{1}{2} e^{-(s+1)}$$

Exact solution (on $[a, b] = [0, 1]$, $\lambda = \frac{1}{2}$): $y(s) = e^{-s}$

Further Applications

Validation of numerical output

intpakX validation of results:



Further Applications

Validation of numerical computations

**Taylor coefficients of the solution with Klein's integral equation solver
(Pascal SC, 1990):**

- 0: $[-2.237925152851349E + 001, -2.237925152851302E + 001]$
- 1: $[-2.066096970005443E + 001, -2.066096970005398E + 001]$
- 2: $[8.243606353500635E - 001, 8.243606353500650E - 001]$
- 3: $[2.747868784500211E - 001, 2.747868784500217E - 001]$
- 8: $[4.089090453125313E - 005, 4.089090453125323E - 005]$
- 15: $[1.260804150517788E - 012, 1.260804150517793E - 012]$

Verified Taylor coefficients of the exact solution (intpakX):

- 0: $[-2.237925152851318850067467E + 001, -2.237925152851318850067128E + 001]$
- 1: $[-2.066096970005414326531422E + 001, -2.066096970005414326531125E + 001]$
- 2: $[8.243606353500640734243249E - 001, 8.243606353500640734243261E - 001]$
- 3: $[2.747868784500213578081081E - 001, 2.747868784500213578081088E - 001]$
- 8: $[4.089090453125317824525419E - 005, 4.089090453125317824525428E - 005]$
- 15: $[1.260804150517790180352184E - 012, 1.260804150517790180352188E - 012]$

Further Applications

Multiple Precision Interval Arithmetic

Maple's arbitrary precision arithmetic + intpakX = Multiple precision Interval arithmetic

Only a limited number of environments offer multiple precision and intervals at the same time, e.g.

- MPFI or GMP-(X)SC (arbitrary precision, both based on the GNU multiple precision library), C-XSC (fixed multiple precision („staggered“)) and some others.

→ Maple other type of environment

Further Applications

Multiple Precision Interval Arithmetic

Comparison

Different objectives:

- Libraries for C++-like standard programming languages
 - Efficient programs, but possibly time-consuming implementation of algorithms.
- Maple-like environments (offering symbolical computing and a GUI)
 - Convenient environment with additional graphics capabilities and easy programming, but lack of efficiency.

Further Applications

Multiple Precision Interval Arithmetic

Timing - Some numbers

Standard functions ([intpakX](#))

	10000 Digits	20000 Digits	40000 Digits	100000 Digits
$\sin(x)$	14.62	57.25	196.95	1586.5
$\exp(x)$	3.28	12.21	46.59	249.05

Standard functions ([GMP-XSC](#))

	10000 Digits	20000 Digits	40000 Digits	100000 Digits
$\sin(x)$	2.50	9.80	39.44	225.47
$\exp(x)$	1.15	4.63	17.81	103.38

Further Applications

Multiple Precision Interval Arithmetic

Timing - Some numbers

Standard functions (Maple float vs. intpakX)

(Times for 1000 iterations)

	Maple float (90 Digits)	intpakX int. (90 Digits)	ratio
$\sin(x)$	4.63	19.42	4.1
$\sinh(x)$	2.74	4.71	1.7
$\exp(x)$	2.60	4.20	1.6

Availability/Contact

Available from Waterloo MapleTM as

Maple PowerTool *Interval Arithmetic*

<http://www.mapleapps.com/powertools/interval/Interval.shtml>

or directly from our Research Group's website at

<http://www.math.uni-wuppertal.de/wrswt/software/intpakX/>

Contact: markus.grimmer@math.uni-wuppertal.de