Around the Numerical Evaluation of D-Finite Functions

Marc Mezzarobba

AriC Team – Inria

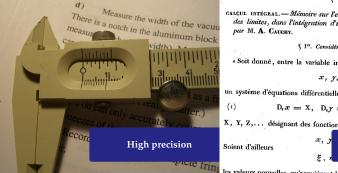


CAPA Seminar, Uppsala universitet June 12, 2012

0.9900	0.42345 08779 18527	0.83850 80695 55370
01	.42336 70387 10965	.83855 04104 51134
02	.42328 32076 37097	.83859 27429 63383
03	.42319 93846 98665	.83863 50670 92932
04	.42311 55698 97410	.83867 73828 40594
0.9905	0.42303 17632 35074	0.83871 96902 07183
06	.42294 79647 13396	.83876 19891 93512
07	.42286 41743 34116	.83880 42798 00397
08	.42278 03920 98971	.83884 65620 28651
09	.42269 66180 09698	.83888 88358 79088
0.9910	0.42261 28520 68035	0.83893 11013 52524
11	.42252 90942 75717	.83897 33584 49774
12	.42244 53446 34478	.83901 56071 71651
13	.42236 16031 46054	.83905 78475 18972
14	.42227 78698 12177	.83910 00794 92552
0.9915 16 17 18 19	0.42219 41446 34579 .42211 04276 1 .42202 67187 5 .42194 30180 5 .42185 93255 2	0.83914 23030 93207 Introduction
0.9920	0.42177 56411 51354	0.83935 32955 31151

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NumGfun

(14)

CALCUL INTÉGRAL. - Mémoire sur l'emploi du nouveau calcul appelé calcul des limites, dans l'intégration d'un système d'équations différentielles; par M. A. CAUCHY.

§ I^{er}. Considérations générales.

« Soit donné, entre la variable indépendante t et les inconnues

x, y, z, ...,

un système d'équations différentielles de la forme

(1) $D_t x = X$, $D_t y = Y$, $D_t z = Z$,...,

x, y

٤

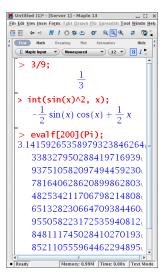
X, Y, Z,... désignant des fonctions connues de

Soient d'ailleurs

Bounds

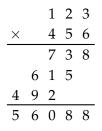
0.9900	0.42345 08779 18527	0.83850 80695 55370
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0.9920	0.42177 56411 51354	0.83935 32955 31151

Computer Algebra

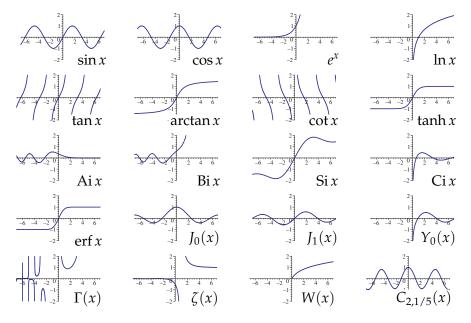


- exact + arbitrary precision computations "symbolic" tools
- computational complexity
- objects: polynomials, matrices... this talk: special functions
- symbolic-numeric algorithms accuracy issues → links with rigorous computing

Complexity: Fast Multiplication



- ► Θ(n²) is not the best possible [Karatsuba, 1963]
- ► One can multiply two integers of ≤ *n* bits in O(n log n 2^{O(log* n)}) bit ops [Fürer 2007].



D-Finite Functions

An analytic function $y(z) : \mathbb{C} \to \mathbb{C}$ is said to be D-finite (holonomic) iff it satisfies a linear (homogeneous) ODE with polynomial coefficients:

$$a_r(z) y^{(r)}(z) + \dots + a_1(z) y'(z) + a_0(z) y(z) = 0, \quad a_j \in \mathbb{K}[z].$$

The sequence of Taylor coefficients of a D-finite functions obeys a linear *recurrence relation* with polynomial coefficients.

Example: $y(z) = \sin z$ y''(z) + y(z) = 0 y(0) = 0, y'(0) = 1

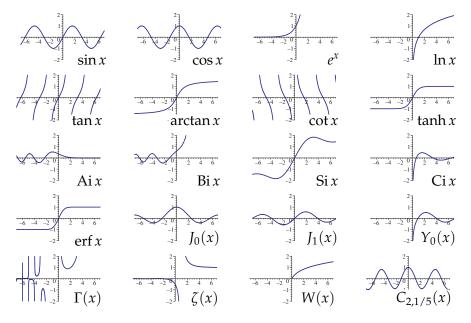
D-Finite Functions

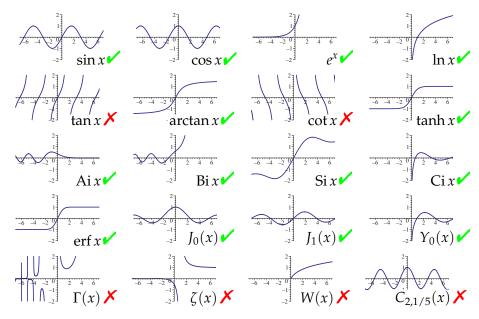
An analytic function $y(z) : \mathbb{C} \to \mathbb{C}$ is said to be D-finite (holonomic) iff it satisfies a linear (homogeneous) ODE with polynomial coefficients:

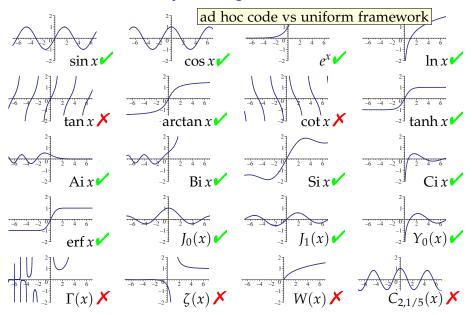
 $a_r(z) y^{(r)}(z) + \dots + a_1(z) y'(z) + a_0(z) y(z) = 0, \quad a_j \in \mathbb{K}[z].$

The sequence of Taylor coefficients of a D-finite functions obeys a linear *recurrence relation* with polynomial coefficients.

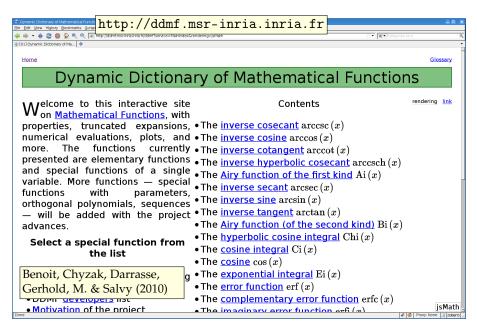
Example : $y(z) = K_0(z)$ (modified Bessel function) z y''(z) + y'(z) - z y(z) = 0

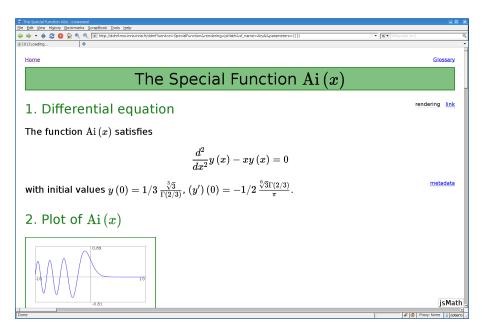


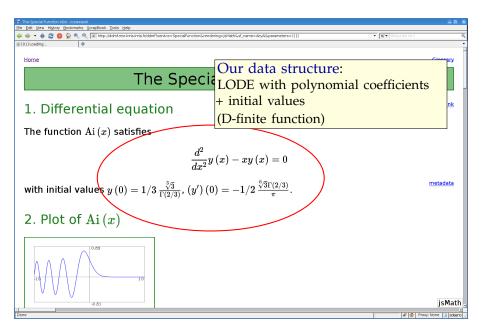


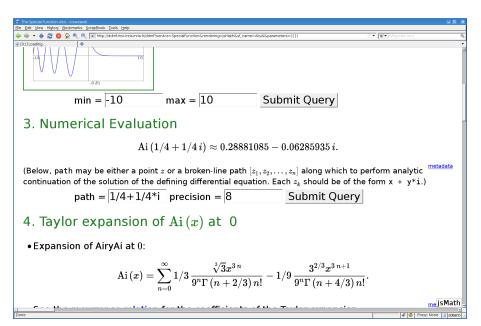


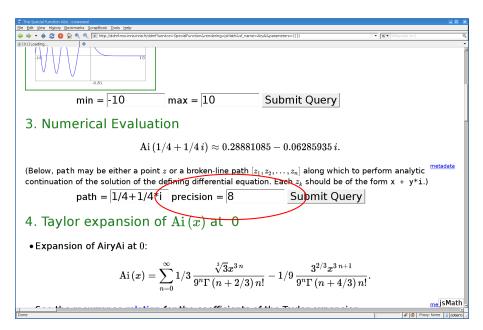
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Edit View Higtory Bookmarks ScrapBook Tools Help						
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01) Dynamic Dictionary of Ma						
Home		Glossary				
Dynamic Dictionary of Mathematical Functions						
valecome to this interactive site	Contents	rendering link				
W ^{elcome} to this interactive site on <u>Mathematical Functions</u> , with	contents					
properties, truncated expansions,	• The inverse cosecant $\arccos(x)$					
numerical evaluations, plots, and						
more. The functions currently	• The inverse cotangent $\operatorname{arccot}(x)$					
presented are elementary functions	• The inverse hyperbolic cosecant $\operatorname{arccsch}(x)$					
and special functions of a single	• The Airy function of the first kind $Ai(x)$					
variable. More functions — special	• The inverse secant $\operatorname{arcsec}(x)$					
functions with parameters,	• The inverse sine $\arcsin(x)$					
orthogonal polynomials, sequences						
min be duded man the project	• The inverse tangent $\arctan(x)$					
	• The <u>Airy function (of the second kind)</u> $\operatorname{Bi}(x)$					
Select a special function from	• The hyperbolic cosine integral $\mathrm{Chi}(x)$					
the list	• The <u>cosine integral</u> $Ci(x)$					
	• The <u>cosine</u> $\cos(x)$					
	• The <u>exponential integral</u> $\operatorname{Ei}(x)$					
nop on selecting and comparing						
5	• The error function $\operatorname{erf}(x)$					
	$ullet$ The $\operatorname{complementary}$ error function $\operatorname{erfc}\left(x ight)$; - N.4.				
• Motivation of the project	The imaginary error function orfi (x)	jsMa				

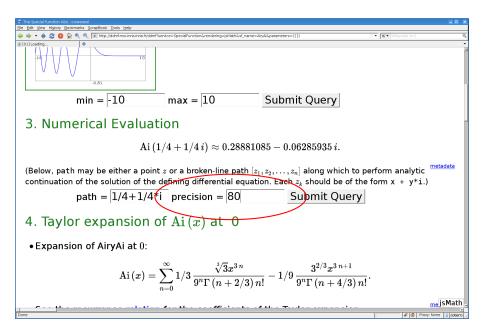


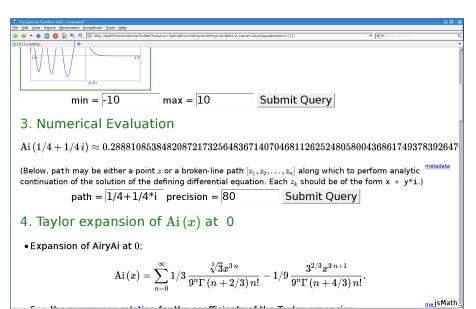




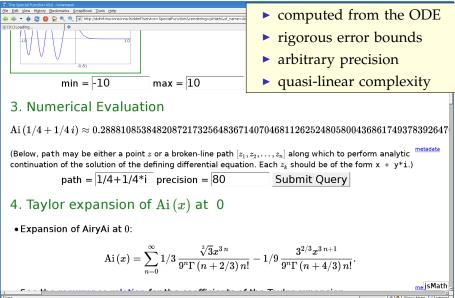




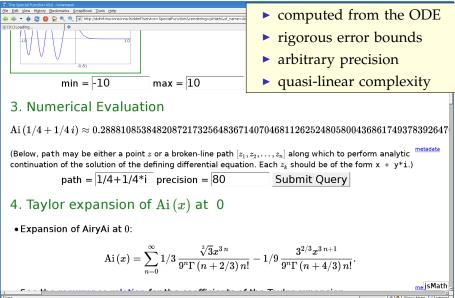


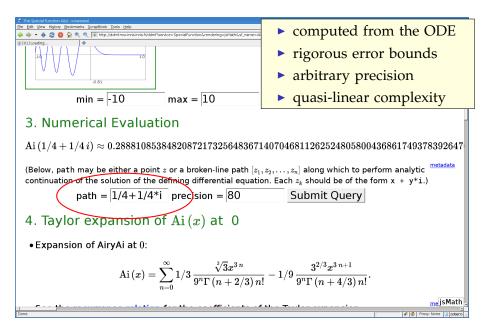


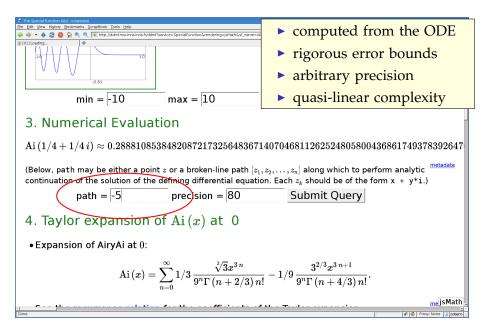
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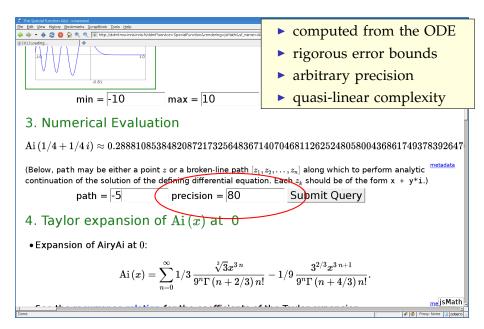


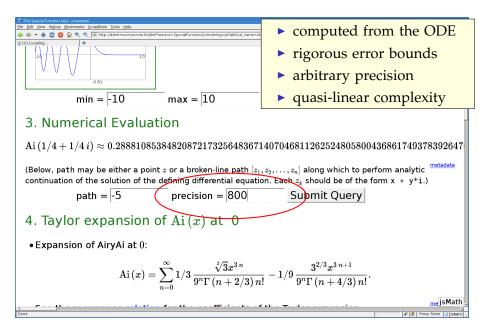
The Special Function Aloci - Iceweasel Ele Edit View Higtory Bookmarks ScrapBook Tools Help	► computed from the ODE
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Storyconder:	 rigorous error bounds
	 arbitrary precision
	 quasi-linear complexity
!36861749378392647020710083742 — 0.06285934655654 form analytic ^{metadata} prm x + y*i.)	5730232761436943988956545624961055148330
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Done	🖓 🙆 Proxy: None 💷 zoteno

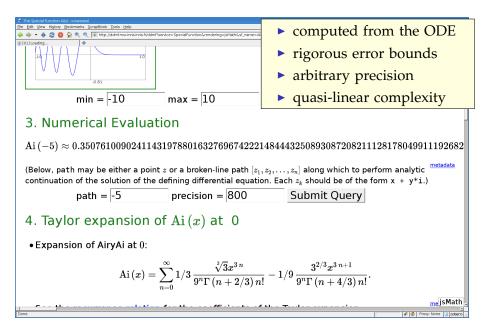












NumGfun

© Bruce Marlin

NumGfun



http://algo.inria.fr/libraries/ (GNU LGPL)

http://algo.inria.fr/libraries/papers/gfun.html



B. Salvy and P. Zimmermann. Gfun: a Maple package for the manipulation of generating and holonomic functions in one variable. ACM TOMS, 1994.

M. Mezzarobba. NumGfun: a Package for Numerical and Analytic Computation with D-finite functions. ISSAC 2010.

M. Mezzarobba. Autour de l'évaluation numérique des fonctions D-finies. PhD thesis, École polytechnique, 2011.

> diffeq := {diff(diff(y(z),z),z)+(2*z^3z^2*a-2*z-a)/((z+1)^2*(z-1)^2)*diff(y(z) ,z)+(z^2*b+z*c+2*z*a+d)*y(z)/((z-1)^3* (z+1)^3),y(0)=1,(D(y))(0)=0};

> diffeq := {diff(diff(y(z),z),z)+(2*z^3-
z^2*a-2*z-a)/((z+1)^2*(z-1)^2)*diff(y(z),
z)+(z^2*b+z*c+2*z*a+d)*y(z)/((z-1)^3*
(z+1)^3),y(0)=1,(D(y))(0)=0};
diffeq := {
$$\frac{d^2}{dz^2}y(z) + \frac{(2z^3-z^2a-2z-a)(\frac{d}{dz}y(z))}{(z+1)^2(z-1)^2} + \frac{(z^2b+zc+2za+d)y(z)}{(z-1)^3(z+1)^3}, y(0) = 1, D(y)(0) = 0$$

>

> diffeq := {diff(diff(y(z),z),z)+(2*z^3-
z^2*a-2*z-a)/((z+1)^2*(z-1)^2)*diff(y(z),
,z)+(z^2*b+z*c+2*z*a+d)*y(z)/((z-1)^3*
(z+1)^3),y(0)=1,(D(y))(0)=0};
diffeq := {
$$\frac{d^2}{dz^2}y(z) + \frac{(2z^3-z^2a-2z-a)(\frac{d}{dz}y(z))}{(z+1)^2(z-1)^2} + \frac{(z^2b+zc+2za+d)y(z)}{(z-1)^3(z+1)^3}, y(0) = 1, D(y)(0) = 0$$

> a, b, c, d := 1, 1/3, 1/2, 3;

> diffeq := {diff(diff(y(z),z),z)+(2*z^3-
z^2*a-2*z-a)/((z+1)^2*(z-1)^2)*diff(y(z)
,z)+(z^2*b+z*c+2*z*a+d)*y(z)/((z-1)^3*
(z+1)^3),y(0)=1,(D(y))(0)=0};
diffeq := {
$$\frac{d^2}{dz^2}y(z) + \frac{(2z^3-z^2a-2z-a)(\frac{d}{dz}y(z))}{(z+1)^2(z-1)^2}$$

 $+ \frac{(z^2b+zc+2za+d)y(z)}{(z-1)^3(z+1)^3}, y(0) = 1, D(y)(0) = 0$
> a, b, c, d := 1, 1/3, 1/2, 3;
 $a, b, c, d := 1, \frac{1}{3}, \frac{1}{2}, 3$

Accuracy Issues

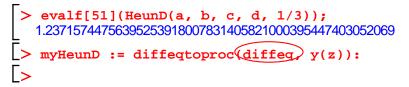
> evalf[51](HeunD(a, b, c, d, 1/3));

Accuracy Issues

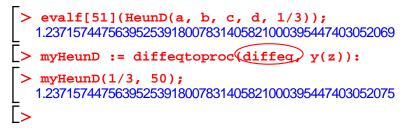
> evalf[51](HeunD(a, b, c, d, 1/3)); 1.23715744756395253918007831405821000395447403052069 >

Accuracy Issues

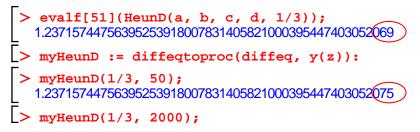
> evalf[51](HeunD(a, b, c, d, 1/3)); 1.23715744756395253918007831405821000395447403052069



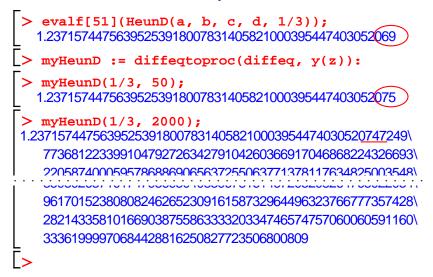
> evalf[51](HeunD(a, b, c, d, 1/3)); 1.23715744756395253918007831405821000395447403052069 > myHeunD := diffeqtoproc(diffeq, y(z)): > myHeunD(1/3, 50);

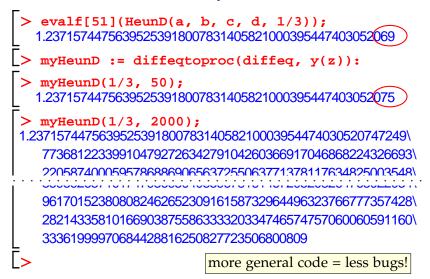


```
> evalf[51](HeunD(a, b, c, d, 1/3));
1.23715744756395253918007831405821000395447403052069
> myHeunD := diffeqtoproc(diffeq, y(z)):
> myHeunD(1/3, 50);
1.23715744756395253918007831405821000395447403052075
>
```



```
> evalf[51](HeunD(a, b, c, d, 1/3));
1.23715744756395253918007831405821000395447403052069
> myHeunD := diffeqtoproc(diffeq, y(z)):
> myHeunD(1/3, 50);
1.23715744756395253918007831405821000395447403052075
> myHeunD(1/3, 2000);
(1.3 s later...)
```

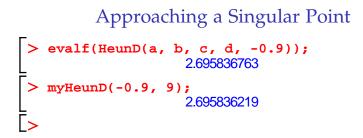


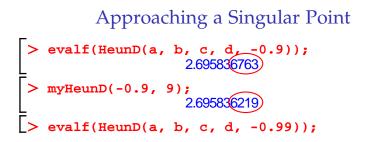


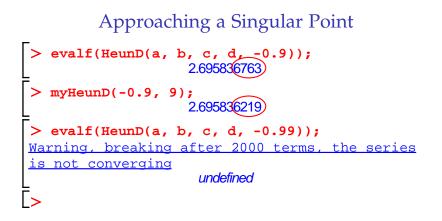
Approaching a Singular Point

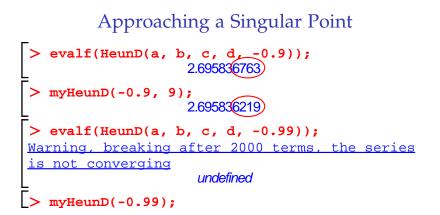
> evalf(HeunD(a, b, c, d, -0.9));

Approaching a Singular Point









```
Approaching a Singular Point
  evalf(HeunD(a, b, c, d, -0.9));
                   2.695836763
> myHeunD(-0.9, 9);
                   2.695836219
> evalf(HeunD(a, b, c, d, -0.99));
Warning, breaking after 2000 terms, the series
is not converging
                     undefined
> myHeunD(-0.99);
                   4.6775585280
```

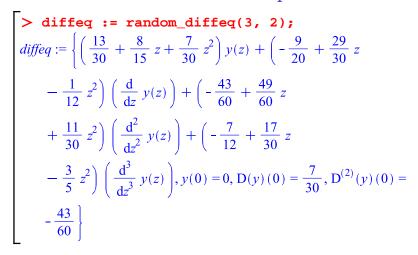
```
Approaching a Singular Point
  evalf(HeunD(a, b, c, d, -0.9));
                   2.695836763
> myHeunD(-0.9, 9);
                   2.6958362
> evalf(HeunD(a, b, c, d, -0.99));
Warning, breaking after 2000 terms, the series
is not converging
                     undefined
> myHeunD(-0.99);
                   4.6775585280
 myHeunD(-0.99, 500);
```

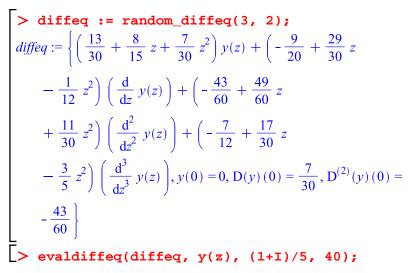
```
Approaching a Singular Point
  evalf(HeunD(a, b, c, d, -0.9));
                    2.695836763
> myHeunD(-0.9, 9);
                    2.6958362
> evalf(HeunD(a, b, c, d, -0.99));
Warning, breaking after 2000 terms, the series
is not converging
                     undefined
> myHeunD(-0.99);
                   4.6775585280
 myHeunD(-0.99, 500);
(6.1 s later...)
```

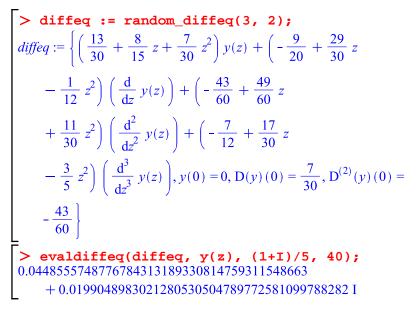
```
Approaching a Singular Point
  evalf(HeunD(a, b, c, d, -0.9));
                    2.695836763
  myHeunD(-0.9, 9);
                     2.695836
> evalf(HeunD(a, b, c, d, -0.99));
Warning, breaking after 2000 terms, the series
is not converging
                      undefined
> myHeunD(-0.99);
                    4.6775585280
> myHeunD(-0.99, 500);
4.677558527966890481646371616414130565650323560409922037
   89542201276207762696563032189351846152496641167932588
   4660460023972873078881
```

```
Approaching a Singular Point
  evalf(HeunD(a, b, c, d, -0.9));
                     2.695836763
  myHeunD(-0.9, 9);
                     2.695836
> evalf(HeunD(a, b, c, d, -0.99));
Warning, breaking after 2000 terms, the series
is not converging
                      undefined
> myHeunD(-0.99);
                    4.6775585280
> myHeunD(-0.99, 500);
4.67755852796689048164637161641413056565032356040992203
   89542201276207762696563
                        no numerical instability issues
   4660460023972873078881
                        (price to pay: computation time)
```

> diffeq := random_diffeq(3, 2);







High Precision

> evaldiffeq(diffeq, y(z), 1/5, 1000000);

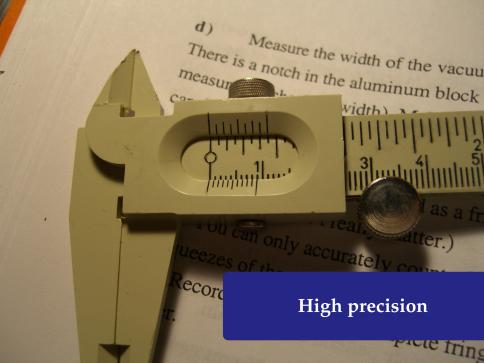
High Precision

> evaldiffeq(diffeq, y(z), 1/5, 1000000); (29 min later...)

High Precision

evaldiffeq(diffeq, y(z), 1/5, 1000000); 0.033253281257567506772459381920024394391065961347292863\ 13611785593075654371610784719859620906805710762776061\ 65993844793918297941976188620650536691082179149605904\ 31080482988558239935175505111768194891591740446771304\ 74730251896359727561534310095807343639273056518962333\ 97217595138842309884016425632431029577130431472108646\ 95485154767624024297343851584414126056237771911489680\

97933258259972366466573219602501650218139747781157348\ 78322628655747195818205282428148240800376913561455564\ 29598794491231828039584256430669932365880956101719727\ 33806130243940574539991121877851105270752378138422728\ 76176859592508040781771637205060431902227437673286901\ 71292574098466950906705927590030494460150099288210121\ 868701569

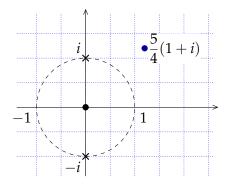


Some Previous Work

- Schroeppel (1972) Special evaluation points
- Brent (1976) Special case of exp (+ variants)
- Chudnovsky & Chudnovsky (1986-1988) General method (incl. a sketch of the case of regular singular points)
- van der Hoeven (1999, 2001) General algorithm with error bounds
- M. Implementation, efficiency improvements, fully automatic error control based on tighter bounds

- 0 fast integer multiplication
- 1 binary splitting

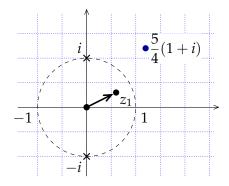
- 2 analytic continuation
- 3 bit burst
- 2. Taylor series method for ODEs



$$\arctan\left(\frac{5}{4}(1+i)\right) = ?$$

- 0 fast integer multiplication
- 1 binary splitting

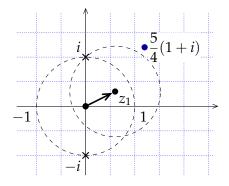
- 2 analytic continuation
- 3 bit burst
- 2. Taylor series method for ODEs



$$\arctan\left(\frac{5}{4}(1+i)\right) = ?$$
$$\begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix} = \begin{bmatrix} 1 & 0.570 \dots + 0.220 \dots i \\ 0 & 0.728 \dots - 0.206 \dots i \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

- 0 fast integer multiplication
- 1 binary splitting

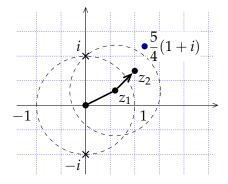
- 2 analytic continuation
- 3 bit burst
- 2. Taylor series method for ODEs



$$\arctan\left(\frac{5}{4}(1+i)\right) = ?$$
$$\begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix} = \begin{bmatrix} 1 \ 0.570 \dots + 0.220 \dots i \\ 0 \ 0.728 \dots - 0.206 \dots i \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

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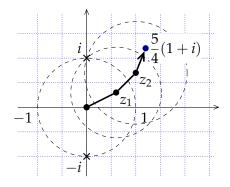
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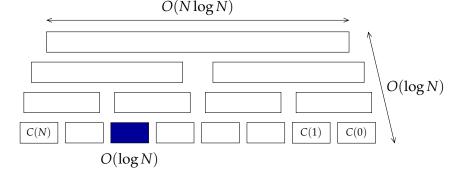
- 0 fast integer multiplication
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- 0. One can multiply two integers of $\leq n$ bits in $M(n) = O(n \log n 2^{O(\log^* n)})$ bit ops [Fürer 2007].

Main Ideas

- 0 fast integer multiplication
- 1 binary splitting

- 2 analytic continuation
- 3 bit burst
- 1. Within the disk of convergence of a Taylor expansion: fast series summation algorithm based on the recurrence



Main Ideas

- 0 fast integer multiplication
- 1 binary splitting

- 2 analytic continuation
- 3 bit burst
- 3. High-precision inputs: use analytic continuation even if the series converges!

$$z_{0} = 10_{2} \rightarrow z_{1} = 10,1_{2}$$

$$\rightarrow z_{2} = 10,101_{2} \qquad \sin(e) = \sin(2,718...) = ?$$

$$\rightarrow z_{3} = 10,1011011_{2}$$

$$\rightarrow z_{4} = 10,101101110010100_{2}$$

$$\rightarrow ...$$

$$\rightarrow z = 10.10110111001010000.....2 \simeq e$$

Main Ideas

- 0 fast integer multiplication
- 1 binary splitting

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- 3 bit burst

Theorem (Chudnovsky²)

The evaluation point *z* being fixed, one may compute y(z) with error bounded by 2^{-n} in

$$O\left(M\left(n\cdot(\log n)^3\right)\right)$$

bit operations.

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The evaluation point z being fixed, one may compute y(z) with error bounded by 2^{-n} in

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bit operations using O(n) bits of memory.

M. Mezzarobba. A note on the space complexity of fast D-finite function evaluation. CASC 2012 (to appear).

Improvements Towards A Practical Algorithm

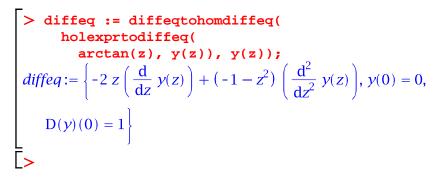
Error control

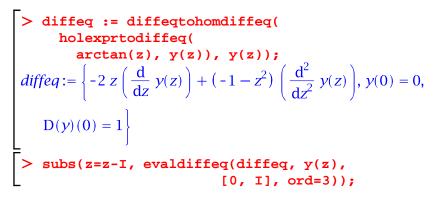
- Precision of intermediate steps
- Tight a priori bounds on truncation orders

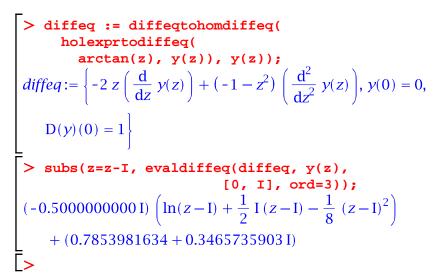
"Constant factor"

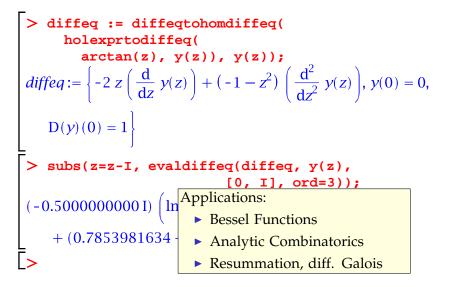
- Structure of recurrence matrices
- Fast simultaneous computations of several derivatives

- "Operator version" of the Heffter-Poole method
- Specific binary splitting algorithm (faster in "hard" cases)









(14)

CALCUL INTÉGRAL. — Mémoire sur l'emploi du nouveau calcul appelé calcul des limites, dans l'intégration d'un système d'équations différentielles; par M. A. CAUCHY.

§ Ier. Considérations générales.

« Soit donné, entre la variable indépendante t et les inconnues

x, y, z, ...,

Bounds

un système d'équations différentielles de la forme

(1)
$$D_t x = X, D_t y = Y, D_t z = Z, \dots,$$

x, y

٤,

X, Y, Z,... désignant des fonctions connues de

Soient d'ailleurs

les valeurs nouvelles qu'acquièrent les in au

Motivation (I): Numerical Evaluation

$$\sum_{n=0}^{\infty} y_n z^n = \sum_{n=0}^{N-1} y_n z^n + \underbrace{\sum_{n=N}^{\infty} y_n z^n}_{2}$$

Compute suitable truncation orders (and other bounds)? A priori bounds tend to be easier to use in fast algorithms.

Chudnovsky & Chudnovsky – Orders of magnitude only
 van der Hoeven (1999, 2001, 2003) – Cauchy-like bounds

We look for asymptotically optimal bounds

Motivation (II): Symbolic Bounds

Baxter Permutations

(OEIS A001181)

►
$$(n+2)(n+3)B_n = (7n^2 + 7n - 2)B_{n-1} + 8(n-1)(n-2)B_{n-2},$$

 $B_0 = B_1 = 1$

►
$$B_n \leq 2,9 \cdot 8^n$$

Chudnovsky Formula for π

$$\begin{aligned} \bullet \quad & \frac{1}{\pi} = \frac{12}{640320^{3/2}} \sum_{k=0}^{\infty} t_k \\ & \text{where} \quad t_k = \frac{(-1)^k (6k)! (13591409 + 545140134k)}{(3k)! (k!)^3 640320^{3k}} \\ \bullet \quad & \left| \frac{640320^{3/2}}{12\pi} - \sum_{k=0}^{n-1} t_k \right| \leq 10^6 (2,3n^3 + 13,6n^2 + 25n + 13,6) \alpha^n \\ & \text{where} \quad \alpha = \frac{1}{151931373056000} \simeq 0,66 \cdot 10^{-14} \end{aligned}$$

"Tight" Bounds

Input Recurrence + Initial terms $\{p_s(n) y_{n+s} + \dots + p_0(n) y_n = 0, y_0 = \dots, y_1 = \dots\}$

Output $|y_n| \leq n!^{p/q} \alpha^n \varphi(n)$

 φ subexponential, i.e. $\varphi(n) = e^{o(n)}$

- rigorous bound in all cases
- for generic initial values:
 optimal *p*/*q* and *α* (or even φ(n) = n^{O(1)})

Theorem

One may compute p/q, α , φ fulfilling these conditions.

M. Mezzarobba and B. Salvy. Effective bounds for P-recursive sequences. Journal of Symbolic Computation, 2010.

Symbolic and Numeric Bounds

Bound Parameters $\kappa, \alpha, \ldots \in \mathbb{Q} \text{ or } \overline{\mathbb{Q}} \text{ s.t.}$ $|y_n| \leq n!^{\kappa} \cdot \alpha^n \cdot \varphi(n)$

Main Tools: Cauchy majorants + elementary asymptotic analysis

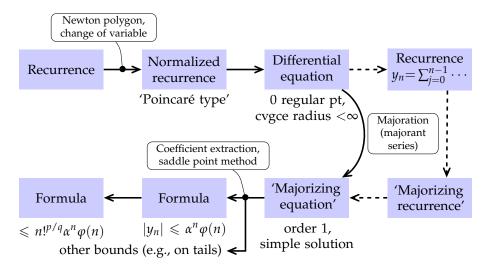
Symbolic Bounds

- Readable (as far as possible!)
- Asymptotically tight

Numeric Bounds

- Safe approx. of parameters
- Faster (no alg. numbers)

Outline of the Algorithm



Impact on Numerical Evaluation

	$\frac{\arccos(z)}{(z^2-1)(z^2+5)}$ @ $\frac{1}{2}$	$\psi(1/2)$	arctan $\frac{9}{10}$	arctan $\frac{99}{100}$
10^{-10}	64/27	40/23	336/164	4238/1496
10^{-100}	380/321	342/313	2338/2108	25210/21848
10^{-1000}	3392/3307	3336/3293	22050/21754	231844/227810
	$\frac{\exp(1/(1-z))}{(1-z)}$ @ $\frac{1}{2}$	$\operatorname{Bi}\left(\frac{1}{1-z}\right)$ @ $\frac{1}{2}$	$\operatorname{Ai}(\frac{1}{1-z})$ @ $\frac{3}{4}$	$\operatorname{Ai}(\frac{1}{1-z})$ @ $\frac{7}{8}$
10^{-10}	70/54	148/56	1558/77	23818/215
10^{-100}	418/387	664/416	3430/879	29258/2025
10^{-1000}	3568/3490	4700/3645	16284/8372	69594/18529
		_		
	e^{-100}	$\operatorname{erf}^2(1)$	$\operatorname{erf}(10)$	$\operatorname{erf}(100)$
10^{-10}	298/291	60/33	628/574	54492/54388
10^{-100}	456/450	190/163	936/894	54904/54800
10^{-1000}	1406/1402	1036/1011	2828/2800	58870/58772

terms: computed / optimal



D-finite functions, DDMF

compute everything we can starting from LODE + ini. cond.

- Multiple Precision Analytic Continuation general – rigorous – fully automatic – fast
- Tight bounds symbolic + numeric – Cauchy majorant method



Code available from

http://algo.inria.fr/libraries/papers/gfun.html



Current & future work

- NumGfun 1.0 and beyond
- Moderate precision, Rigorous polynomial approximations
- Majorants vs enclosures + fixed point thms
- ► D-Finite functions in Computer Arithmetic, code generation



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- http://commons.wikimedia.org/wiki/File: Calipers_in_physics_lab.jpg (by User:Falcorian, Creative Commons Attribution-Share Alike)
- Augustin-Louis Cauchy; Mémoire sur l'emploi du nouveau calcul, appelé calcul des limites, dans l'intégration d'un système d'équations différentielles; *Comptes-rendus de l'Académie des Sciences* 15, 1842 (public domain)
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