Reliable numerical evaluation of special functions. Algorithms and experiments.

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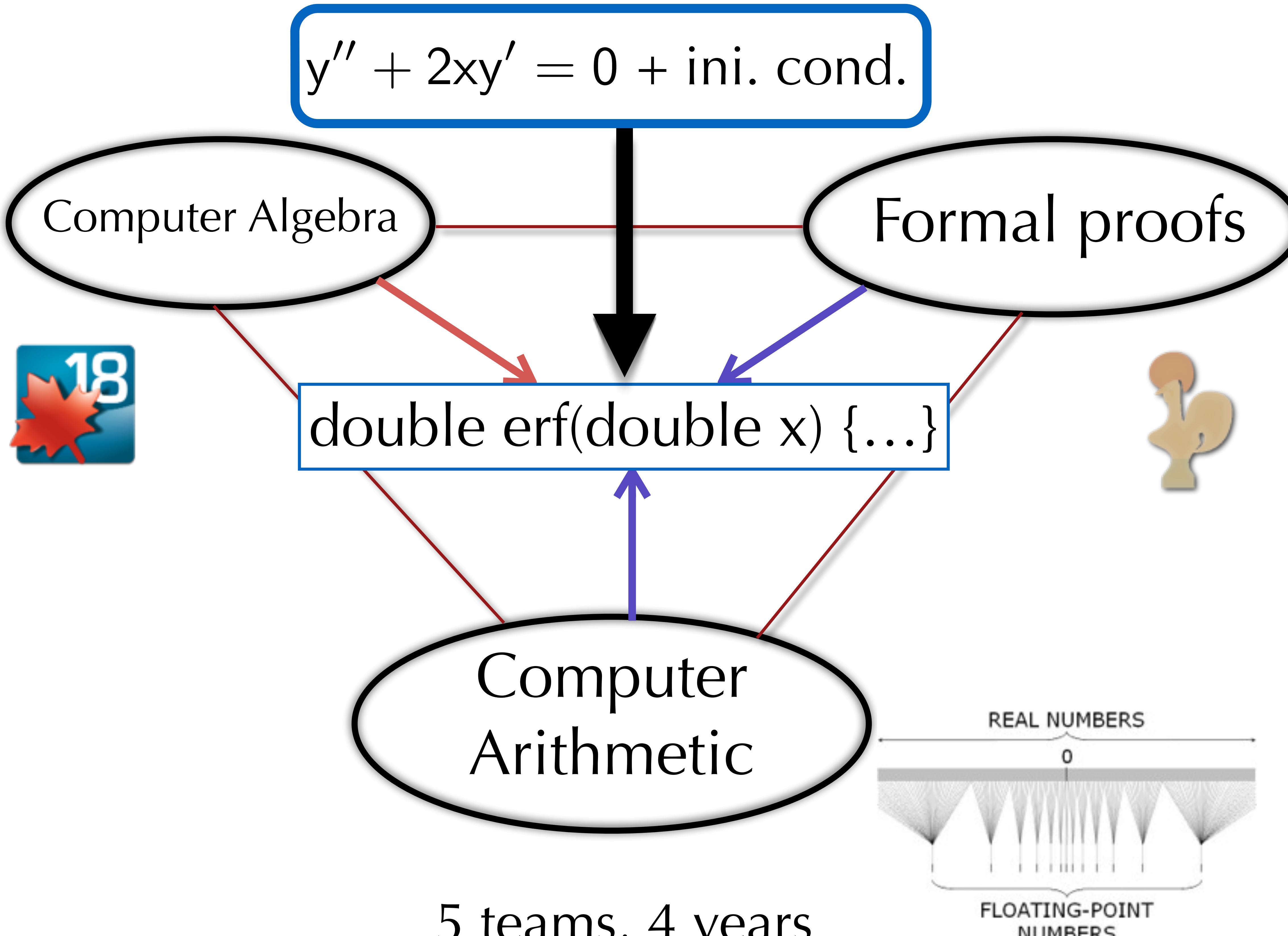
July 21st, 2014

New project: FastRelax (starting this Fall)



5 teams, 4 years

I. Equations as a data-structure

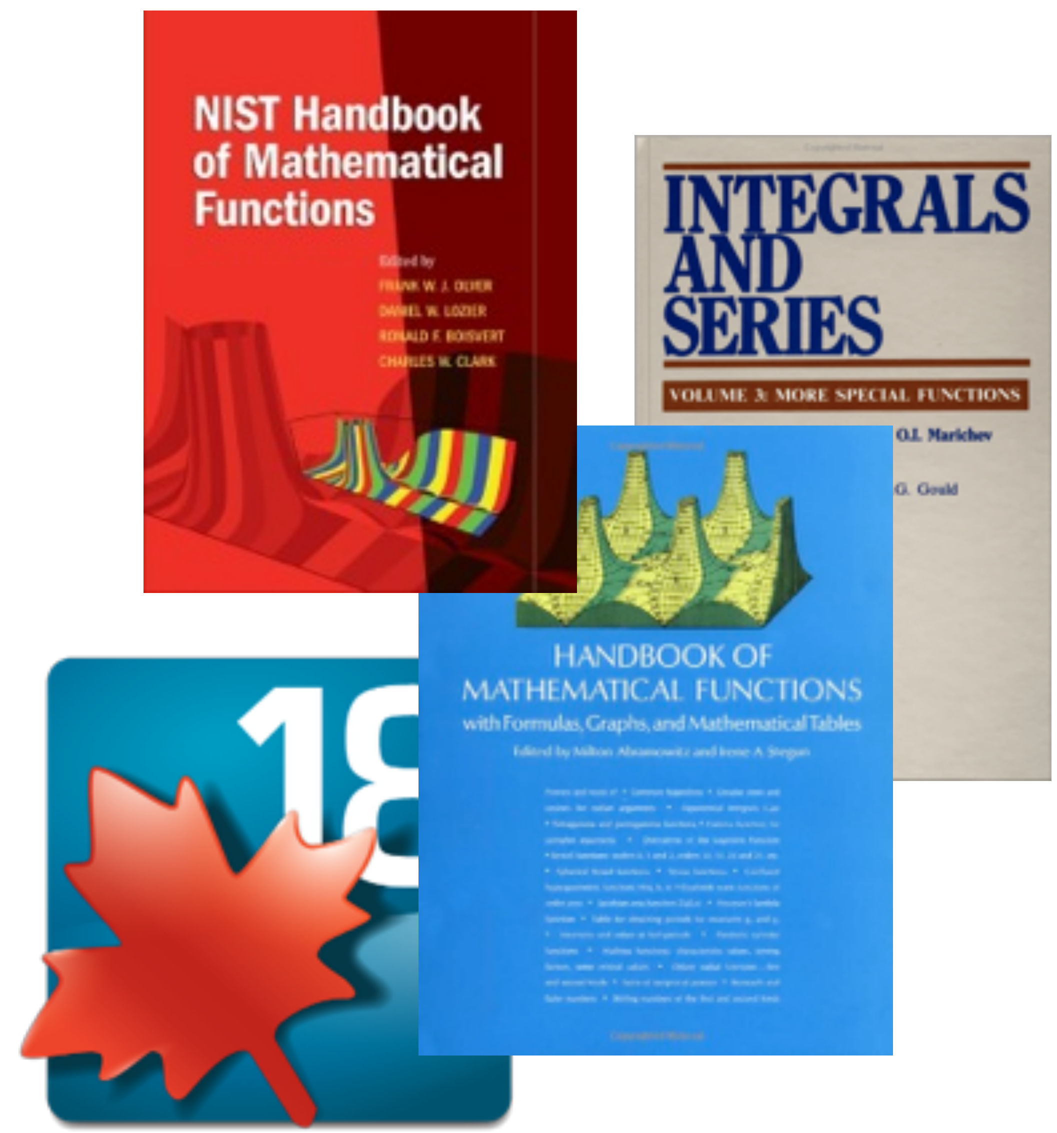
$$\mathrm{erf} := (\mathsf{y}'' + 2\mathsf{xy}' = 0, \text{ini. cond.})$$

basis of the gfun package

Dynamic Dictionary of Mathematical Functions

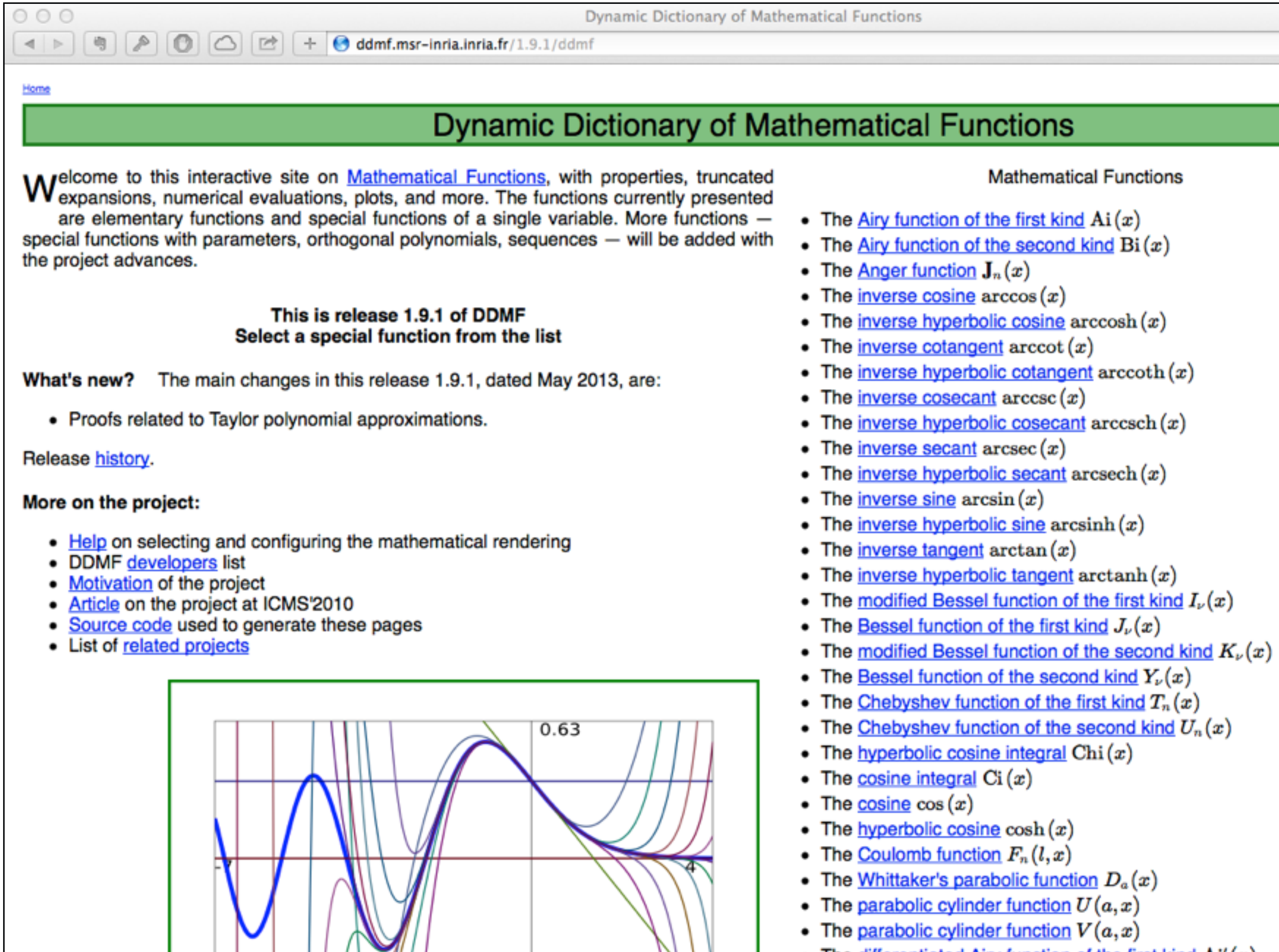
- User need
- Recent algorithmic progress
- Maths on the web

http://ddmf.msr-inria.inria.fr/



Heavy work by F. Chyzak

Demonstration



II. Numerical evaluation via the Taylor series

From large integers to precise numerical values

Numerical evaluation of solutions of LDEs

Principle:
$$f(x) = \underbrace{\sum_{n=0}^{N} a_n x^n}_{\text{fast evaluation}} + \underbrace{\sum_{n=N+1}^{\infty} a_n x^n}_{\text{good bounds}}$$

f solution of a LDE with coeffs in $\mathbf{Q}(x)$ (our data-structure!)

1. linear recurrence in N for the first sum (easy);
2. tight bounds on the tail (e.g., [Mezzarobba,S.2010]);
3. no numerical roundoff errors.

The technique used for fast evaluation of constants like

$$\frac{1}{\pi} = \frac{12}{C^{3/2}} \sum_{n=0}^{\infty} \frac{(-1)^n (6n)!(A + nB)}{(3n)!n!^3 C^{3n}}$$

with A=13591409,
B=545140134,
C=640320.

Code available: [NumGfun] [Mezzarobba 2010]

Binary Splitting for linear recurrences (70's and 80's)

- n! by divide-and-conquer:

$$n! = \underbrace{n \times \cdots \times \lceil n/2 \rceil}_{\text{size } O(n \log n)} \times \underbrace{\lfloor n/2 \rfloor \times \cdots \times 1}_{\text{size } O(n \log n)}$$

Cost: $O(n \log^3 n \log\log n)$ using FFT

- linear recurrences of order 1 reduce to

$$p!(n) := (p(n) \times \cdots \times p(\lceil n/2 \rceil)) \times (p(\lfloor n/2 \rfloor) \times \cdots \times p(1))$$

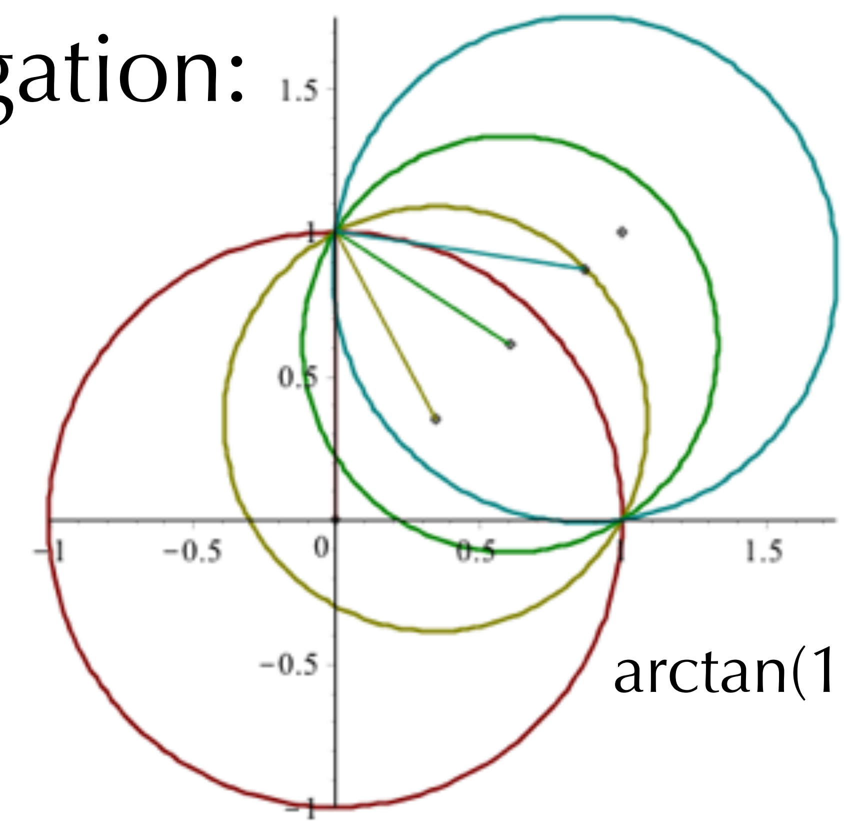
- arbitrary order: same idea, same cost (matrix factorial):

ex $\quad e_n := \sum_{k=0}^{n} \frac{1}{k!}$ satisfies a 2nd order rec, computed via

$$\begin{pmatrix} e_n \\ e_{n-1} \end{pmatrix} = \frac{1}{n} \underbrace{\begin{pmatrix} n+1 & -1 \\ n & 0 \end{pmatrix}}_{A(n)} \begin{pmatrix} e_{n-1} \\ e_{n-2} \end{pmatrix} = \frac{1}{n!} A!(n) \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Analytic continuation

Compute $f(x), f'(x), \ldots, f^{(d-1)}(x)$ as new initial conditions and handle error propagation:



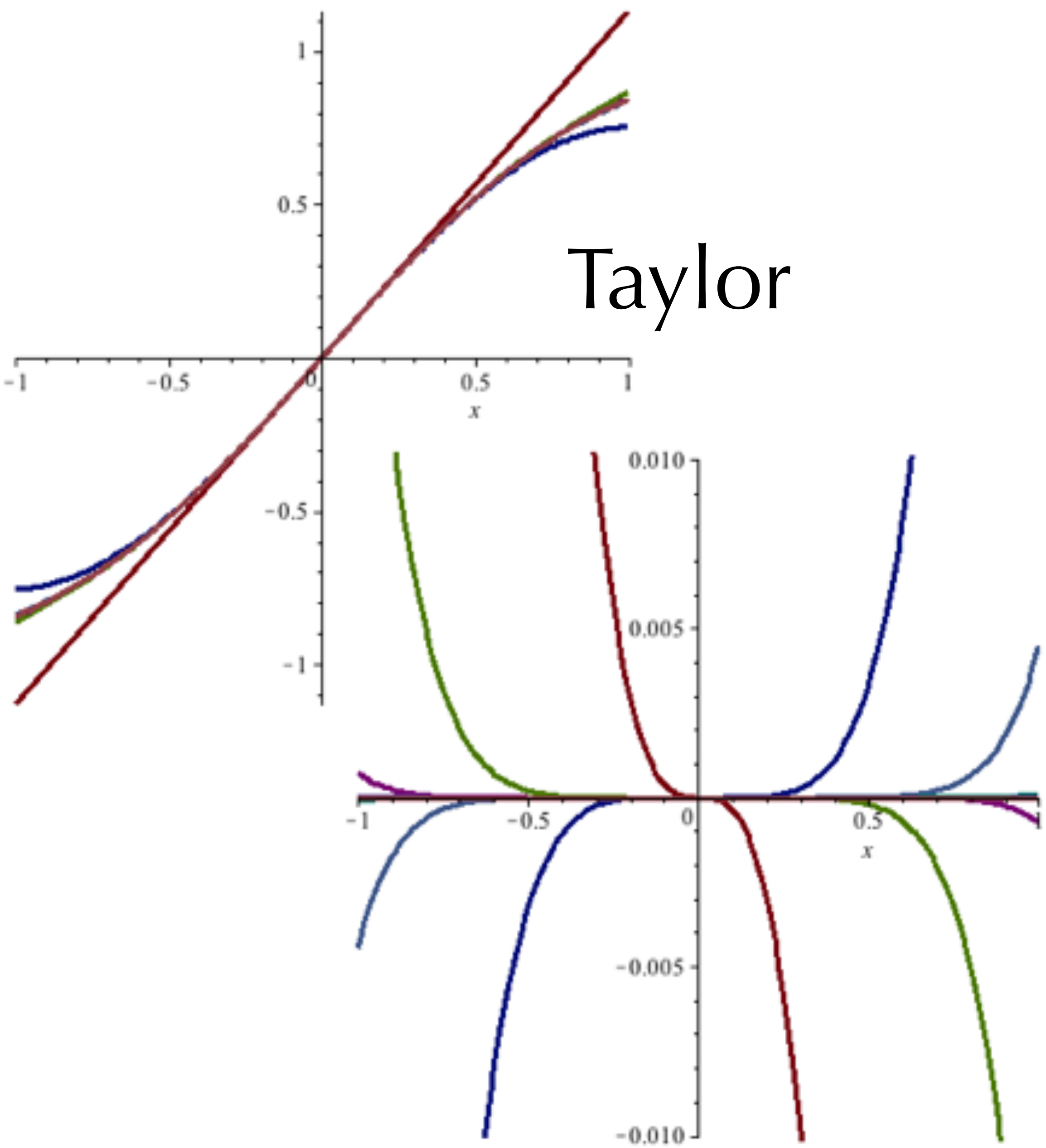
arctan(1+i)

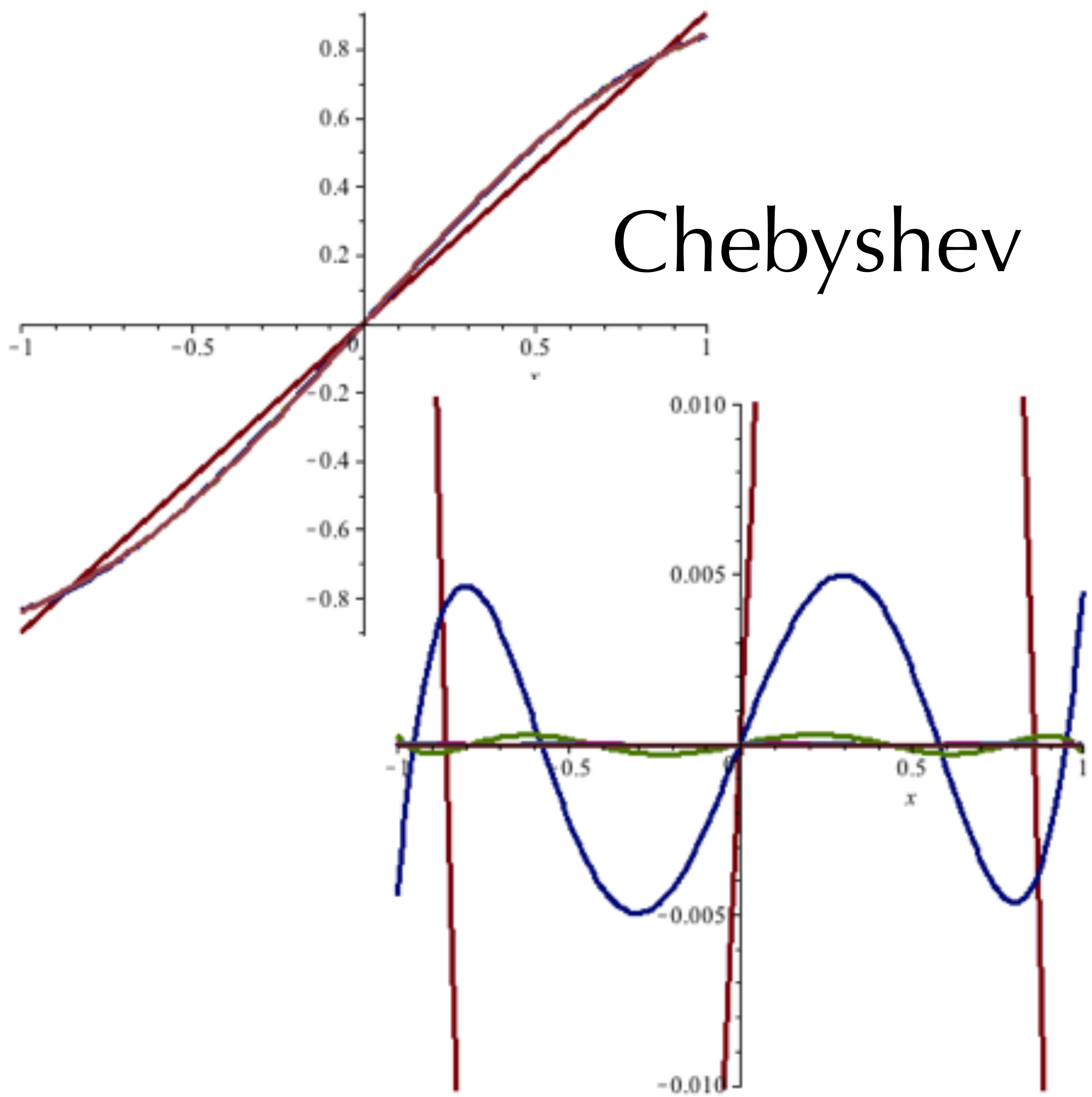
Ex: erf(π) with 15 digits:

$$0 \xrightarrow[\text{200 terms}]{} 3.1416 \xrightarrow[\text{18 terms}]{} 3.1415927 \xrightarrow[\text{6 terms}]{} 3.14159265358979$$

Again: computation on integers. No roundoff errors.

III. Chebyshev expansions





From equations to operators

d/dx ↔ D mult by x ↔ x composition ↔ product $Dx=xD+1$	$(n\mapsto n+1) \leftrightarrow S$ mult by n ↔ n composition ↔ product $Sn=(n+1)S$

Taylor morphism: $D \mapsto (n+1)S$; $x \mapsto S^{-1}$
produces linear recurrence from LDE

erf: $$D^2+2xD \mapsto (n+1)S(n+1)S+2S^{-1}(n+1)S=(n+1)(n+2)S^2+2n$$

Ore (1933): general framework for these non-commutative polynomials.

Main property: deg AB=deg A+deg B.

Consequence 1: (non-commutative) Euclidean division

Consequence 2: (non-commutative) Euclidean algorithm.

Ore fractions ($Q^{-1}P$ with P&Q operators)

Thm. (Ore 1933) Sums and products reduce to that form.

Application: extend Taylor morphism to Chebyshev expansions

Taylor

$x^{n+1}=x\cdot x^n$, $(x^n)'=nx^{n-1}$

$\leftrightarrow X:=S^{-1}$, $D:=(n+1)S$

Chebyshev

$2xT_n(x)=T_{n+1}(x)+T_{n-1}(x)$,

$2(1-x^2)T_n'(x)=-nT_{n+1}(x)+nT_{n-1}(x)$

$\leftrightarrow X:=(S+S^{-1})/2$,

$D:=(1-X^2)^{-1}n(S-S^{-1})/2=2(S^{-1}-S)^{-1}n$.

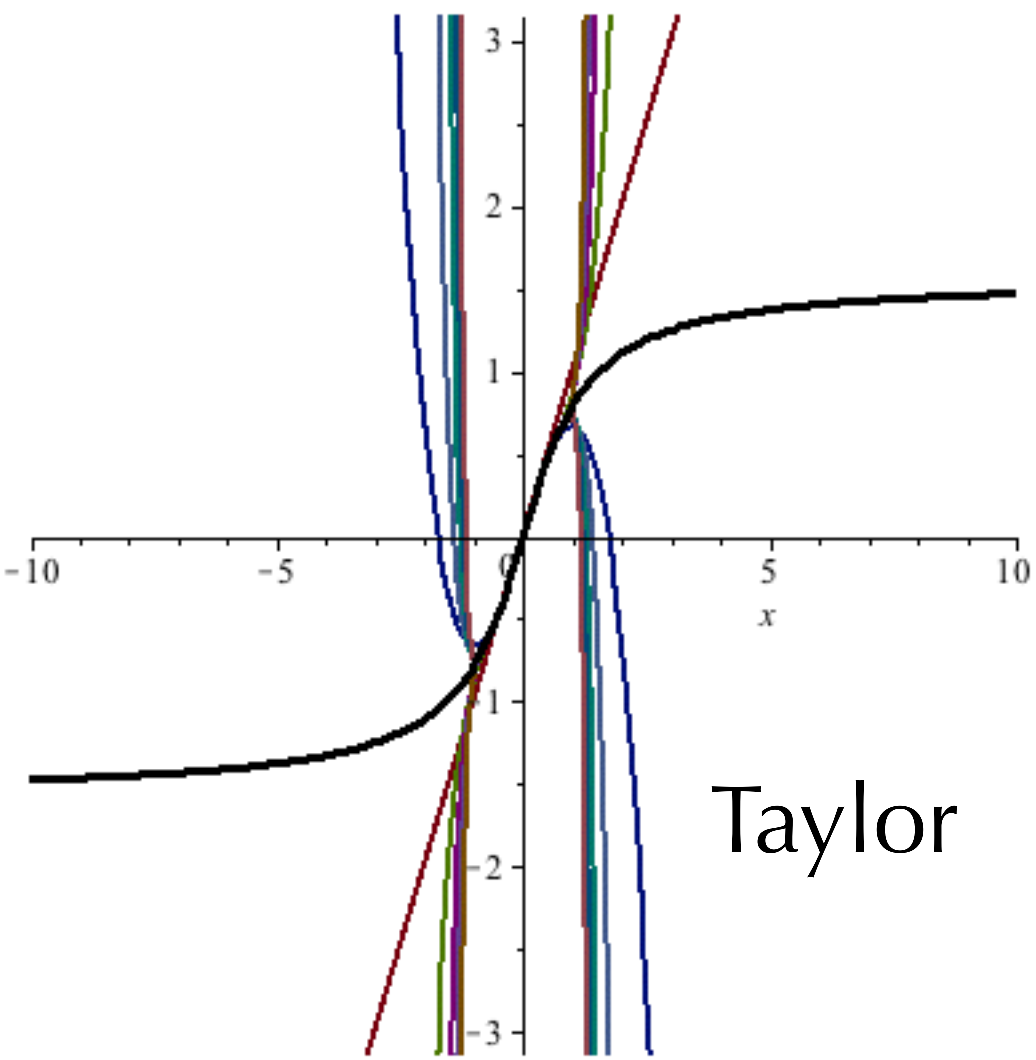
erf: $$D^2+2xD\mapsto(2(S^{-1}-S)^{-1}n)^2+2\frac{S+S^{-1}}{2}2(S^{-1}-S)^{-1}n$$
$$=\mathrm{pol}(n,S)^{-1}(2(n+1)(n+4)S^4-4(n+2)^3S^2+2n(n+3))$$

Prop. [Benoit, S (2009)] If y is a solution of L(x,d/dx), then its Chebyshev coefficients annihilate the numerator of L(X,D).

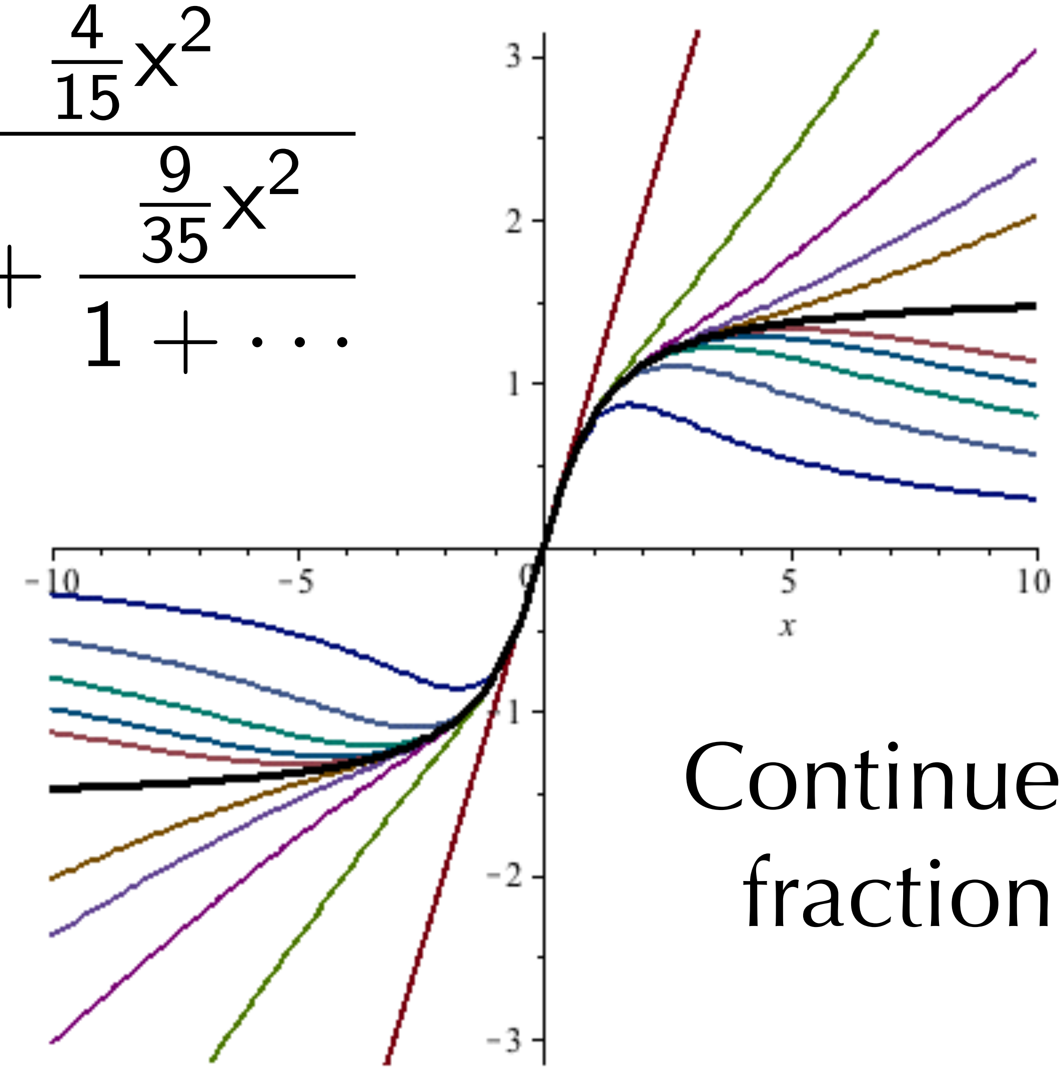
Efficient numerical use: arXiv:1407.2802 (2 weeks ago).

III. Continued Fractions

$$\arctan x = \cfrac{x}{1 + \cfrac{\frac{1}{3}x^2}{1 + \cfrac{\frac{4}{15}x^2}{1 + \cfrac{\frac{9}{35}x^2}{1 + \cdots}}}}$$



Taylor



Continued fraction

A guess & prove approach

(Maulat, S. 2014)

1. Differential equation produces first terms (easy):

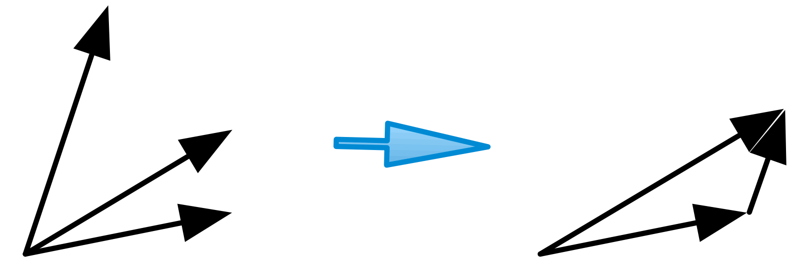
$$\arctan x = \cfrac{x}{1 + \cfrac{\frac{1}{3}x^2}{1 + \cfrac{\frac{4}{15}x^2}{1 + \cfrac{\frac{9}{35}x^2}{1 + \cdots}}}}$$

2. Guess a formula (easy): $a_n = \dfrac{n^2}{4n^2 - 1}$

3. Prove that the CF with these a_n satisfies the differential equation.

No human intervention needed.

Proof technique



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> series(sin(x)^2+cos(x)^2-1,x,4);
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$O(x^4)$

f satisfies a LDE
$\Longleftrightarrow$
f,f',f'',... live in a
finite-dim. vector space

Why is this a proof?

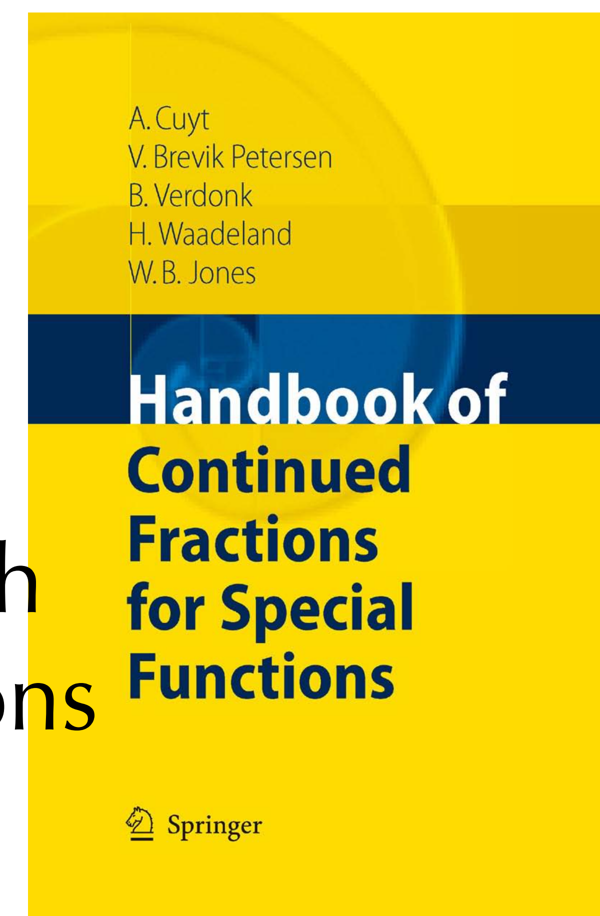
1. sin and cos satisfy a 2nd order LDE: $y''+y=0$;
2. their squares and their sum satisfy a 3rd order LDE;
3. the constant -1 satisfies $y'=0$;
4. thus $\sin^2+\cos^2-1$ satisfies a LDE of order at most 4;
5. Cauchy's theorem concludes.

Proofs of non-linear identities by linear algebra!

Automatic Proof of the guessed CF

$$\arctan x \stackrel{?}{=} \cfrac{x}{1+\cfrac{\cdots}{1+\cfrac{\frac{n^2}{4n^2-1}x^2}{1+\cdots}}}$$

- Aim: RHS satisfies $(x^2+1)y'-1=0$;
- Convergents P_n/Q_n where P_n and Q_n satisfy a LRE (and $Q_n(0)\neq 0$);
- Define $H_n:=(Q_n)^2((x^2+1)(P_n/Q_n)'-1)$;
- H_n is a polynomial in P_n,Q_n and their derivatives;
- therefore, it satisfies a LRE that can be computed;
- from it, $H_n=O(x^n)$ visible, ie lim P_n/Q_n soln;
- conclude $P_n/Q_n\rightarrow$ arctan (check initial cond.).



More generally: this guess-and-proof approach applies to CF for solutions of (q-)Ricatti equations → **all explicit C-fractions** in Cuyt et alii.

Conclusion

- Linear differential equations and recurrences are a great data-structure;
- Numerous algorithms have been developed in computer algebra;
- Efficient code is available;
- More is true (creative telescoping, diagonals,…);
- More to come in DDMF, including formal proofs.

The End