Latest developments in ROOT::Math

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Outline

Restructuring and Extending Mathematical Libraries

1. Revise already implemented functions and algorithms:
   - Testing accuracy, time performance, domains,
   - Crosschecking with well-established implementations: GSL, Mathematica
   - (Re)implementing existing ones.
2. Add useful routines.
3. Provide convenient user interfaces.
4. Reduce dependency on GSL libraries and other ROOT classes (TF1).

What I did

1. New classes for multidimensional integration, using:
   - Adaptive cubature
   - Monte Carlo integration
2. Reimplementation of major special functions and probability distributions
3. On-line documentation (TWiki, upgrade of Inventory), tutorials.

Adaptive cubature

- Checking existing algorithms (ROOT::TF1, TFoam, HintLib)
  - $\longrightarrow$ the best applies Genz-Malik cubature
  - $\longrightarrow$ the best implementation in TF1 class
- Extend functionality of TF1::IntegralMultiple.
  - independence on TF classes and hist library,
  - usage for free functions,
  - and arbitrary number of dimensions (not only 2 or 3).

$\longrightarrow$ IntegralMultiDim class

IntegralMultiDim class - usage

```
ROOT::Math::WrappedParamFunction<> fptr1(&Func, NDim);

ROOT::Math::IntegratorMultiDim ig1;

ig1.SetFunction(fptr1);

ig1.Integral(xmin[], xmax[]);
```

Applying Monte Carlo algorithms

- C++ interface to algorithms from GSL
- MC algorithms for the first time in ROOT (these from RooFit are not universal)
- Good functionality (not restricted to TF objects)

→ GSLMCIntegrator class

The usage of GSLMCIntegrator class

```
ROOT::Math::WrappedParamFunction<> fptr(&Function, NDim);
ROOT::Math::GSLMCIntegrator ig1();
```

Setting algorithm

```
ig1.SetType(ROOT::Math::MCIntegration::VEGAS);
ig1.SetMode(ROOT::Math::MCIntegration::IMPORTANCE);
```

Setting additional parameters

```
VegasParameters param;
param.iterations = 2;
ig1.SetParameters(param);
```

```
ig1.SetFunction(fptr);
ig1.Integral(xmin[], xmax[]);
```

Adaptive Cubature vs Monte Carlo

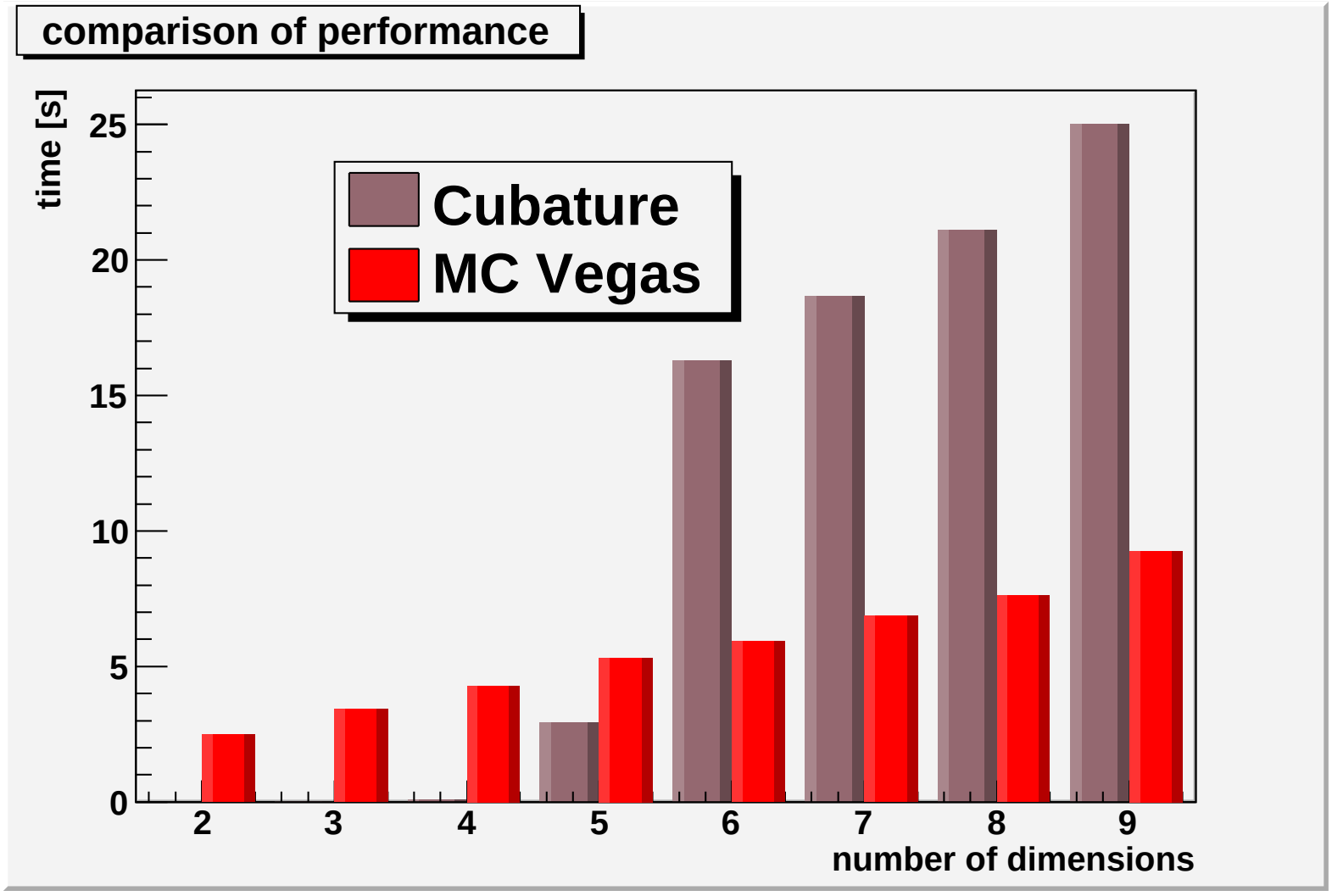
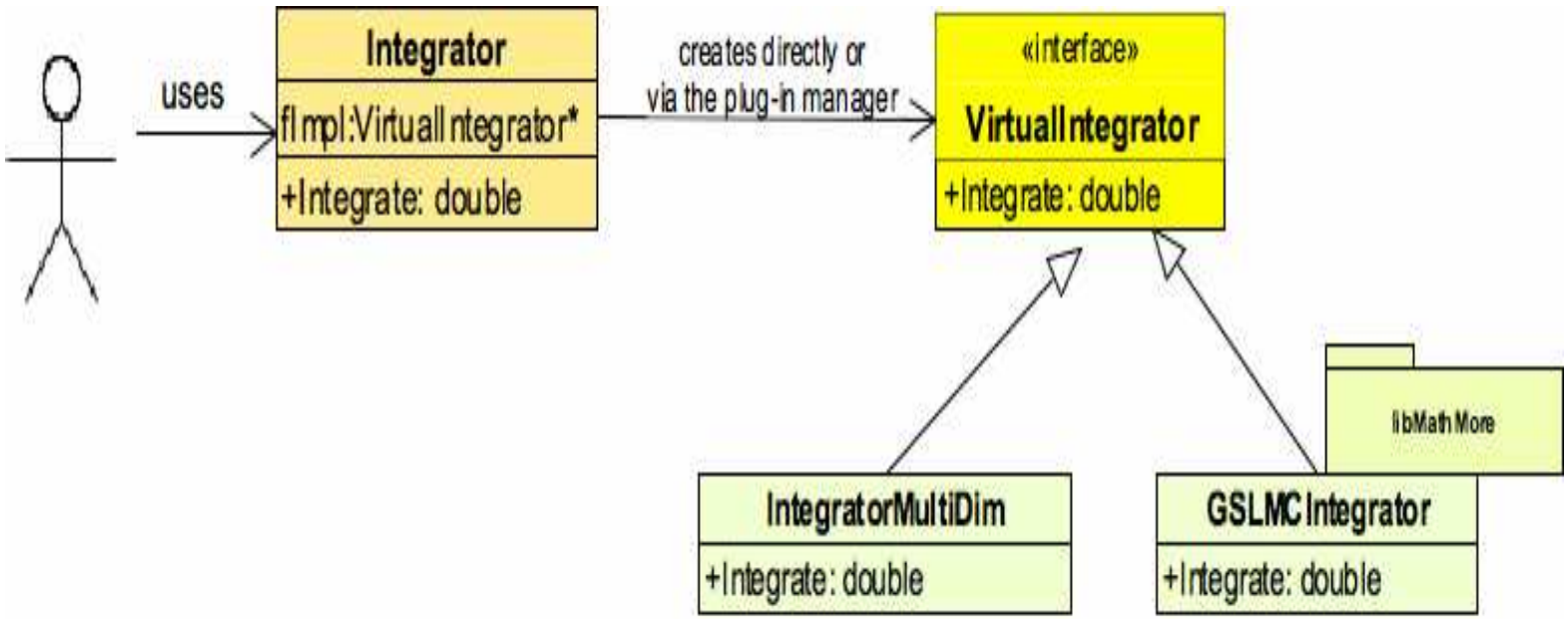


Figure: Achieved accuracy: 0.01

Interface

Using the **plug-in manager** one can load GSL implementation in MathMore



Special functions

Major special functions

- commonly used in physical calculations,
  - (upper) incomplete gamma,
  - incomplete beta
- used for implementing other functions:
  - χ^2 (used in statistical tests performed many times)
  - F- distribution, Student-t distribution, etc (for statistical analysis).

After testing several implementations decided on CEPHES

- free usage netlib
- GSL need license
- NR copywrighted "no transfer or distribution"
- many other pros...

Gamma and related functions

Old TMath

- **Gamma, LnGamma** ▸ Def
- Implementation from NR

New MathCore

- Independent on GSL

Gamma and related functions

Old TMath

- **Gamma, LnGamma** ▸ Def
  - Implementation from NR
  - Domains: $(0, \infty)$

New MathCore

- Independent on GSL
- Domains extended to $(-\infty, \infty) \setminus \mathbb{Z}_-$

Gamma and related functions

Old TMath

- **Gamma, LnGamma** ▸ Def

- Implementation from NR
- Domains: $(0, \infty)$
- Efficiency $11 \cdot 10^{-5}$ (s/100 calls)

▸ gamma comparison

New MathCore

- Independent on GSL
- Domains extended to $(-\infty, \infty) \setminus \mathbb{Z}_-$
- Efficiency $5 \cdot 10^{-5}$ (s/100 calls)

Gamma and related functions

Old TMath

New MathCore

- **Upper incomplete gamma** ▸ Def
- Implementation from NR
- Implementation independent of GSL

Gamma and related functions

Old TMath

New MathCore

- **Upper incomplete gamma** ▸ Def

- Implementation from NR
- Efficiency $11 \cdot 10^{-5}$ (s/100 calls)

- Implementation independent of GSL
- Efficiency $7 \cdot 10^{-5}$ (s/100 calls)

▸ inc gamma comparison

Beta and related functions

Old TMath

- **Beta function** Def

- Beta already implemented in TMath

New MathCore

- Implementation based on CEPHES

Beta and related functions

Old TMath

- **Beta function** ▸ Def

- Beta already implemented in TMath ▸ beta comparison

New MathCore

- Implementation based on CEPHES

Beta and related functions

Old TMath

New MathCore

- **Incomplete Beta** ▸ Def

- Implementation in TMath from NR

- Implementation independent of GSL

Beta and related functions

Old TMath

New MathCore

- **Incomplete Beta** ▸ Def

- Implementation in TMath from NR
- Efficiency $4 \cdot 10^{-4}$(s/100 calls)

- Implementation independent of GSL
- Efficiency $4 \cdot 10^{-4}$(s/100 calls)

Beta and related functions

Old TMath

New MathCore

- **Incomplete Beta** ▸ Def

- Implementation in TMath from NR
- Efficiency $4 \cdot 10^{-4}$(s/100 calls)

▸ inc beta comparison

- Implementation independent of GSL
- Efficiency $4 \cdot 10^{-4}$(s/100 calls)

Error function

Old TMath

- implementation from NR

New MathCore

- from CEPHES library

Error function

Old TMath

- implementation from NR

New MathCore

- from CEPHES library

- Efficiency around 0 better in CEPHES (10%), tails better in TMath (factor 2)

Error function

Old TMath

- implementation from NR

New MathCore

- from CEPHES library

- Efficiency around 0 better in CEPHES (10%), tails better in TMath (factor 2)
- Improvement in accuracy! (single → double precision)

▸ erfc comparison

Probability distributions & cumulatives

Using new implementation of inc_gamma and inc_beta one can reimplement

▸ chi2 comparison ▸ F comparison ▸ Student-t comparison

independently of GSL and NR!

The new implementation in MathCore uses

- base functions from CEPHES library,
- reflexive property for inc_beta function ● to calculate complementary cumulatives

Description & Documentation

An online reconnaissance over Mathematical Libraries:

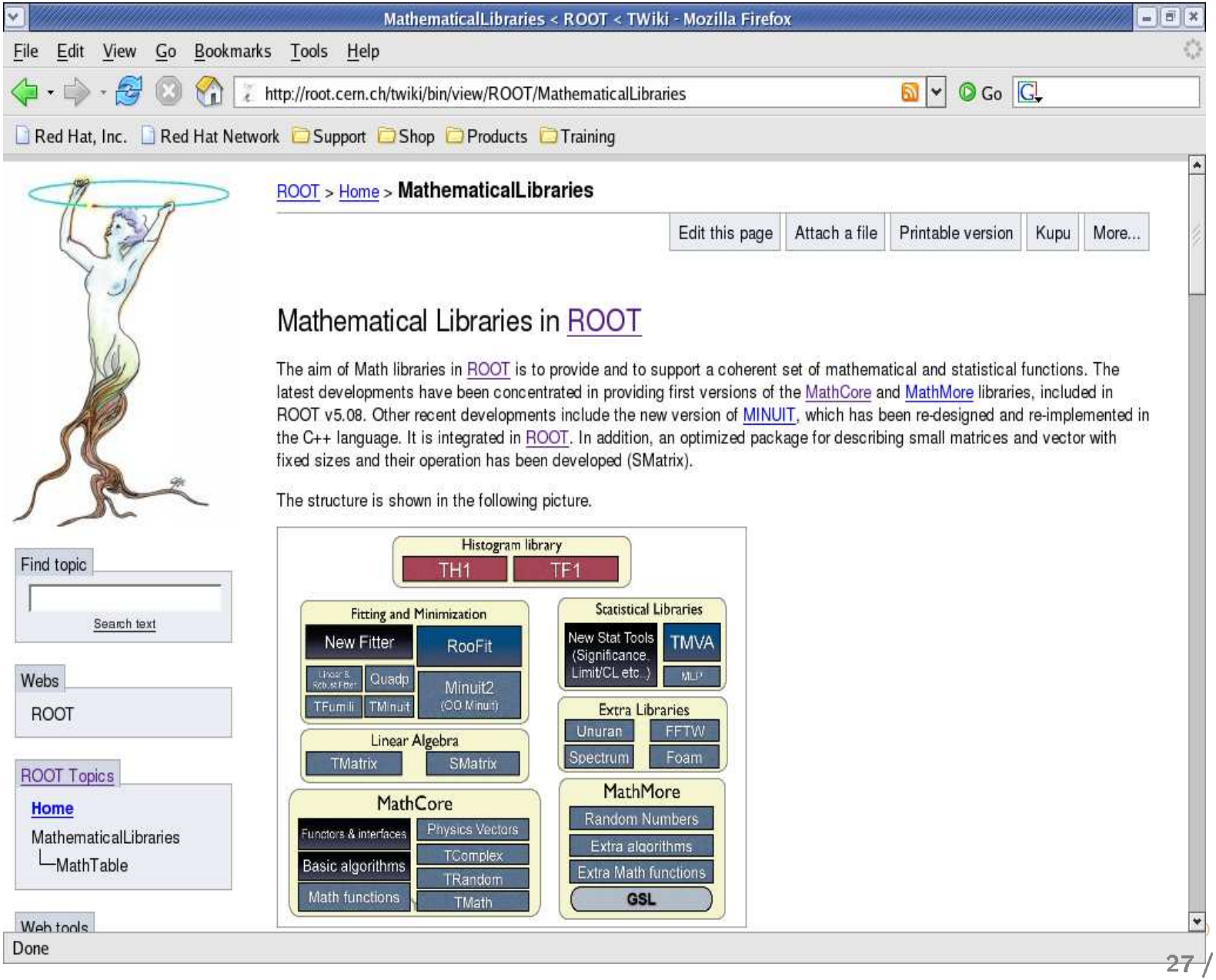
http://root.cern.ch/twiki/bin/view/ROOT/MathematicalLibraries

Information about existing algorithms and functions:

http://root.cern.ch/twiki/bin/view/ROOT/MathTable

Reference to be found at:
ftp://root.cern.ch/root/doc/13MathLibraries.pdf

Mathematical libraries TWiki page



Updated Inventory

MathTable < ROOT < TWiki - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://root.cern.ch/twiki/bin/view/ROOT/MathTable

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ROOT Topics

Home >

MathematicalLibraries

MathTable

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Inventory of Mathematical Functions and Algorithms

LCG Project | LCG Applications Area Cernlib writeup | GSL contents | Abramowitz and Stegun | MathLib Project | Project Portal | $Date: 2007/09/21 15:01:05 $

Functions and Polynomials	Numerical Methods	Random Numbers and Distributions	Others
• Special Functions • Polynomials • Function Approximations	• Integration • Differentiation • Minimization • Root-Finding • Interpolation	• Random Number Generator • Random Number Distribution	• Linear Algebra • Differential Equations • FFT

Special Functions

Routines for evaluating Special functions

Bessel Functions of various types

* **Regular cylindrical functions**	*Bessel J functions of various orders*	ROOT, GSL, Cernlib
* **Irregular cylindrical functions**	*Bessel Y functions of various orders*	ROOT, GSL, Cernlib
* **Regular modified cylindrical**	*Bessel I functions of various orders*	ROOT, GSL, Cernlib
* **Irregular modified cylindrical**	*Bessel K functions of various orders*	ROOT, GSL, Cernlib
* **Regular spherical functions**	*Bessel j functions of various orders*	ROOT, GSL, Cernlib
* **Irregular spherical functions**	*Bessel y functions of various orders*	ROOT, GSL, Cernlib

Examples and tutorials

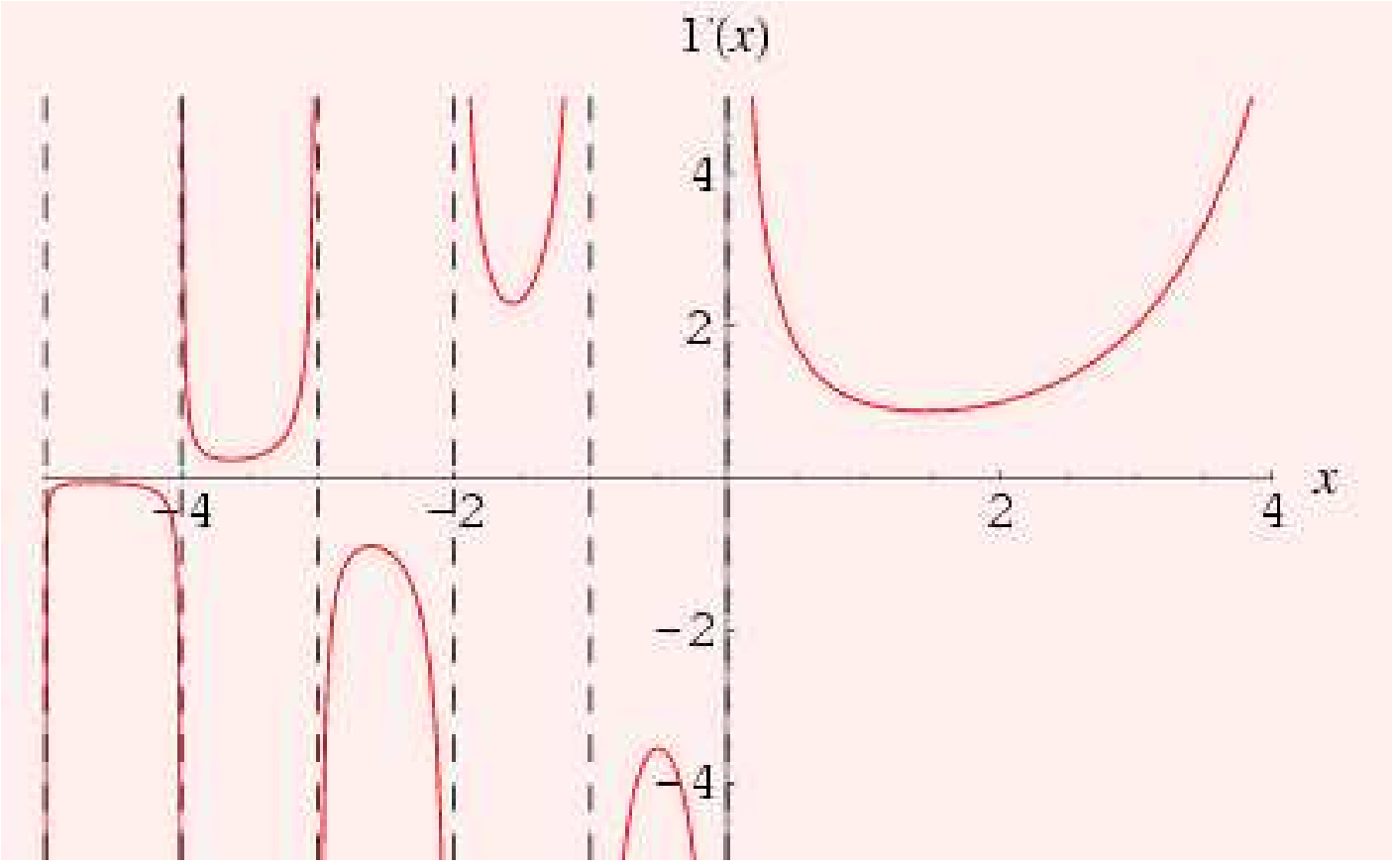
. **Clausen function**	*Clausen integral function*	GSL, Cernlib

The work is done...

Thank You!

gamma function

$$\Gamma(z) \equiv \int_0^\infty dt\ t^{z-1} e^{-t}, \quad a > 0$$



(upper) incomplete gamma function

$$P(a,z) \equiv \frac{1}{\Gamma(a)} \int_0^{\infty} dt\ t^{a-1} e^{-t}, \quad a > 0$$

Back

beta function

$$B(z,w) \equiv \int_0^1 dt\ t^{z-1}(1-t)^{w-1}$$

$$B(z,w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}$$

Back

incomplete beta function

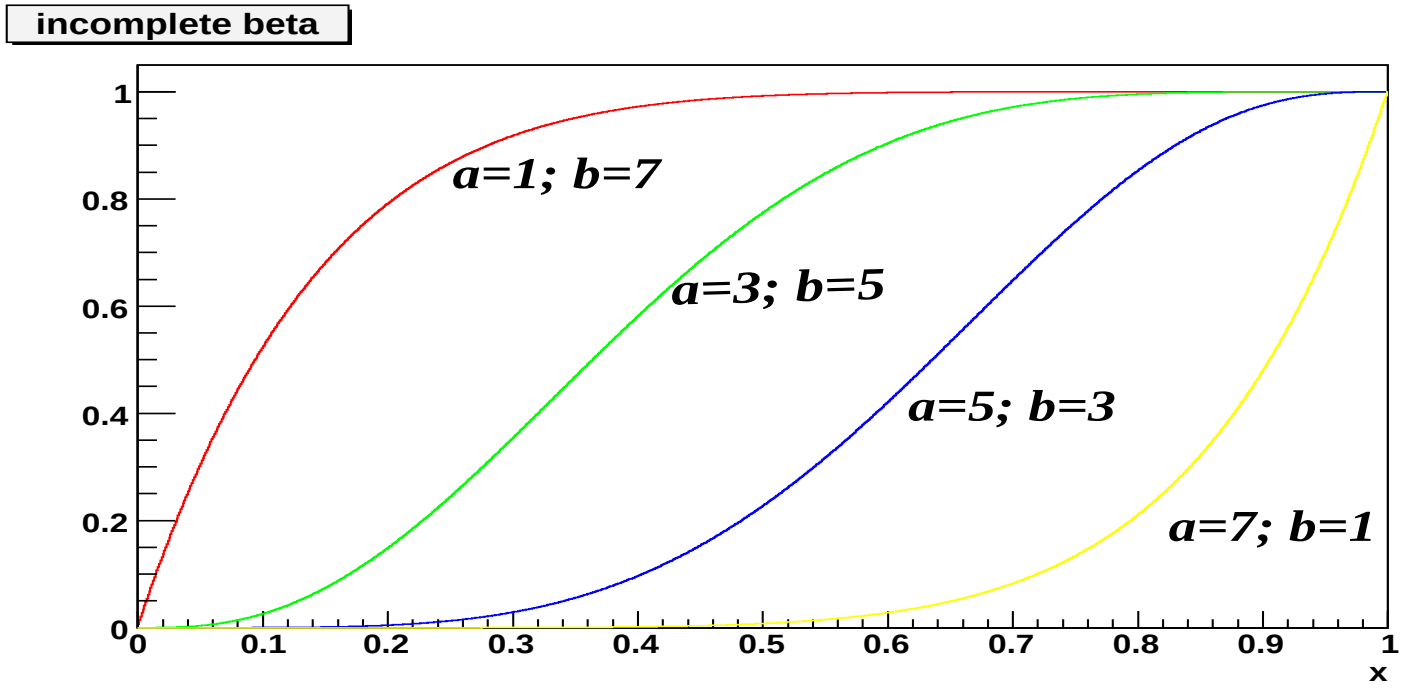


Figure: inc_beta(x, a, b) for different parameters

$$I(x; a, b) \equiv \frac{1}{B(a,b)} \int_0^x dt\ t^{a-1}(1-t^{b-1}) \quad a, b > 0$$

$$\boxed{1 - I(x; a, b) = I(1-x; b, a)}$$

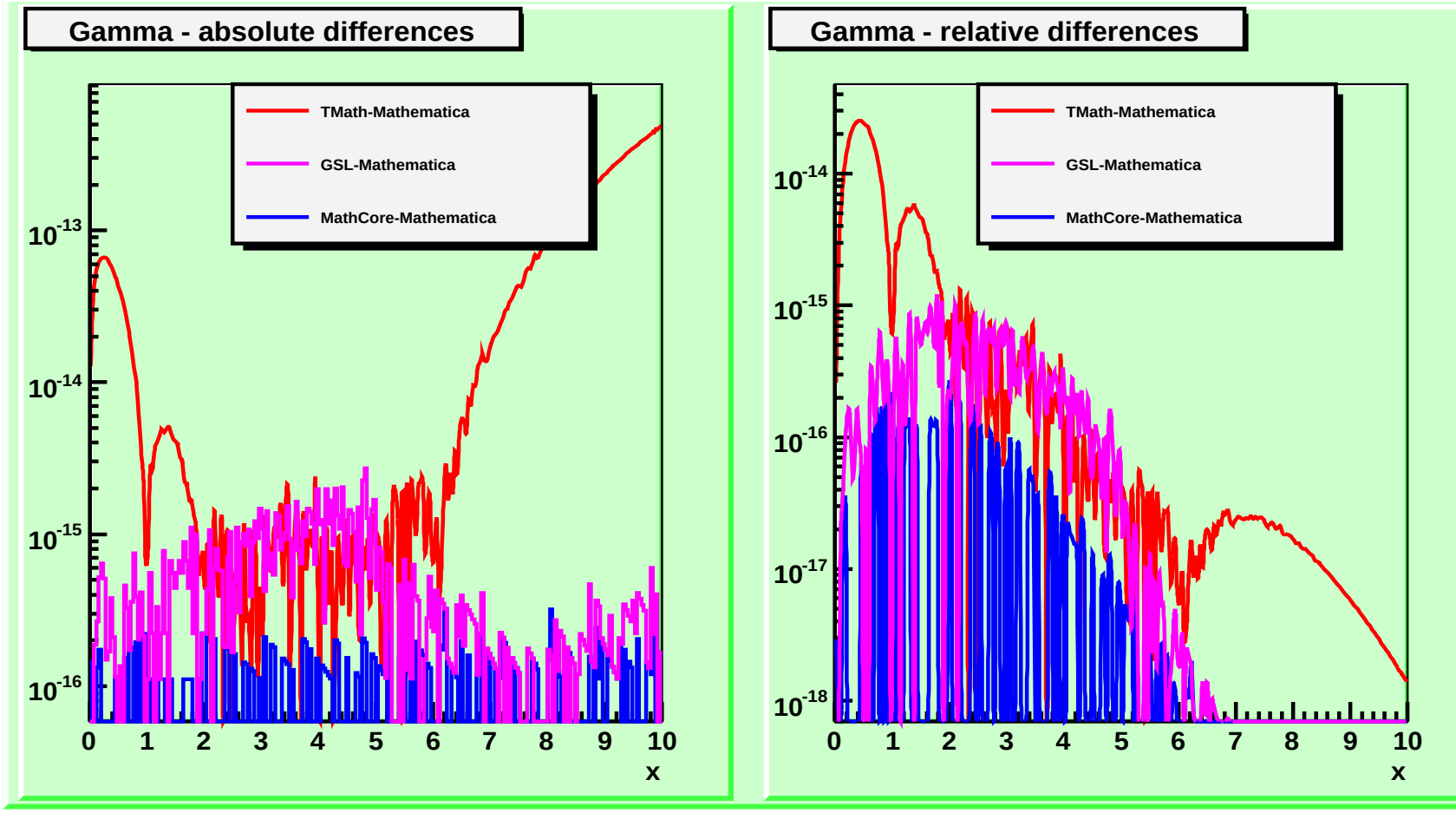


Figure: Comparison with Mathematica Gamma[x]

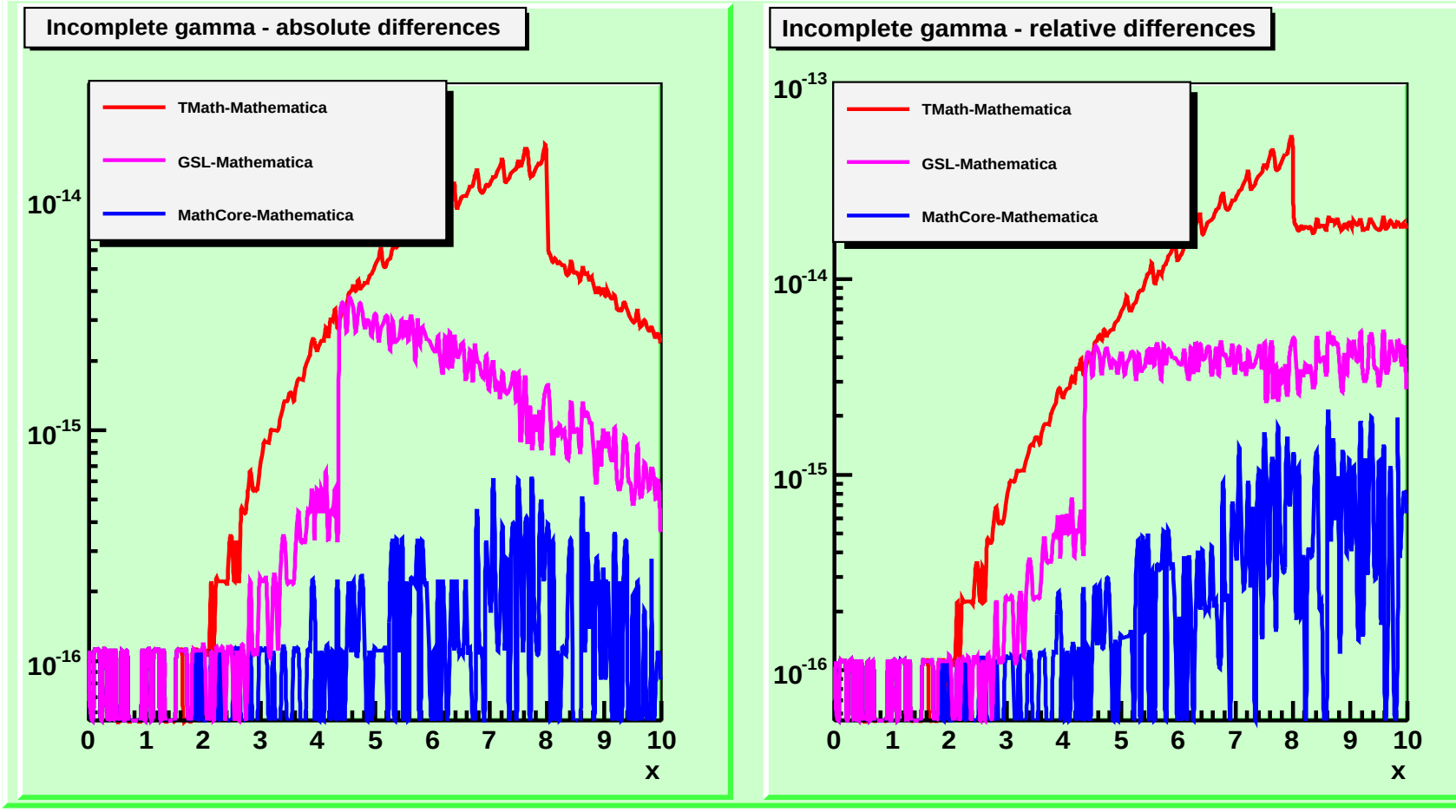


Figure: Comparison with Mathematica GammaRegularized[a, x]

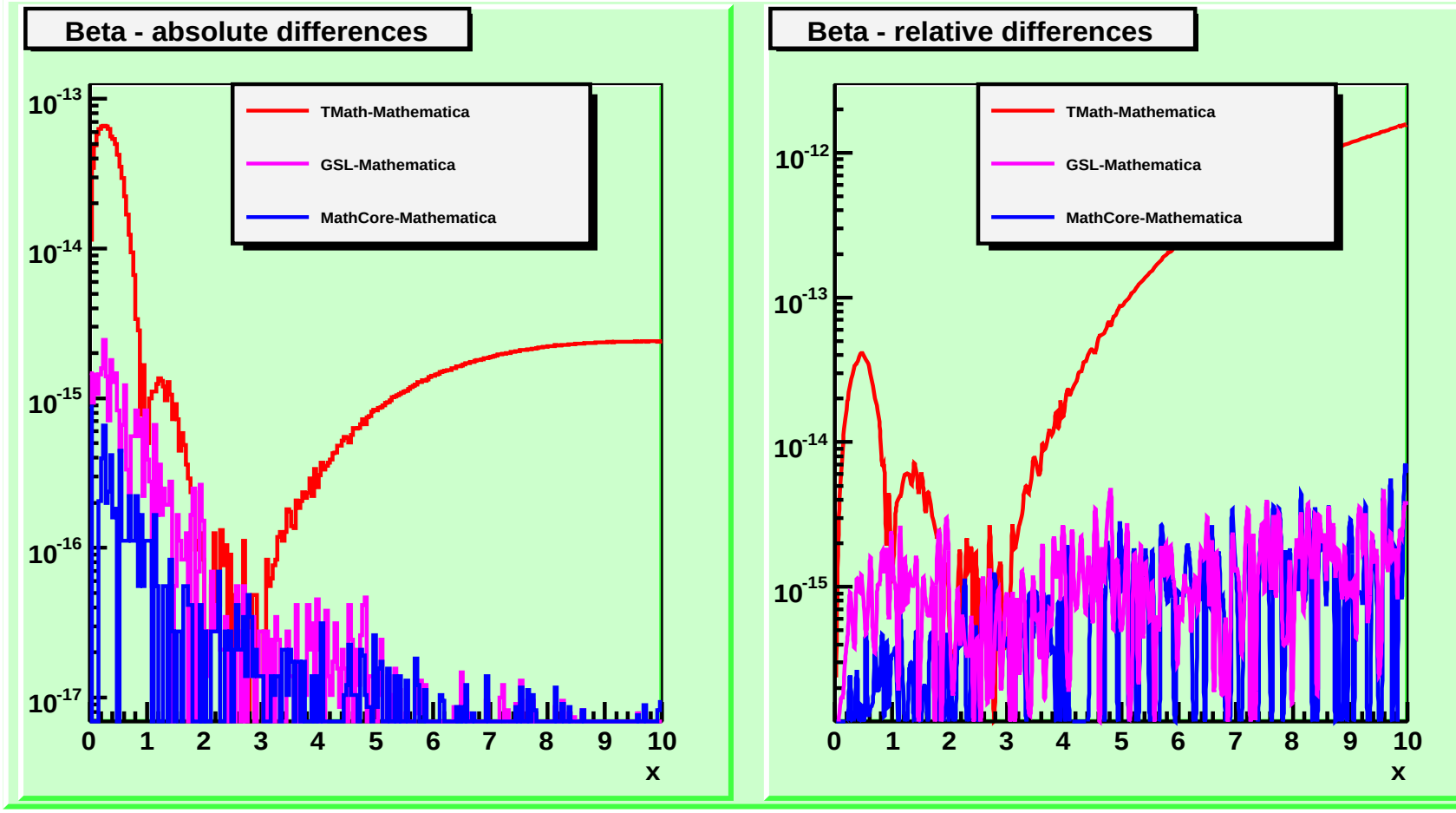


Figure: Comparison with Mathematica Beta[a, x]

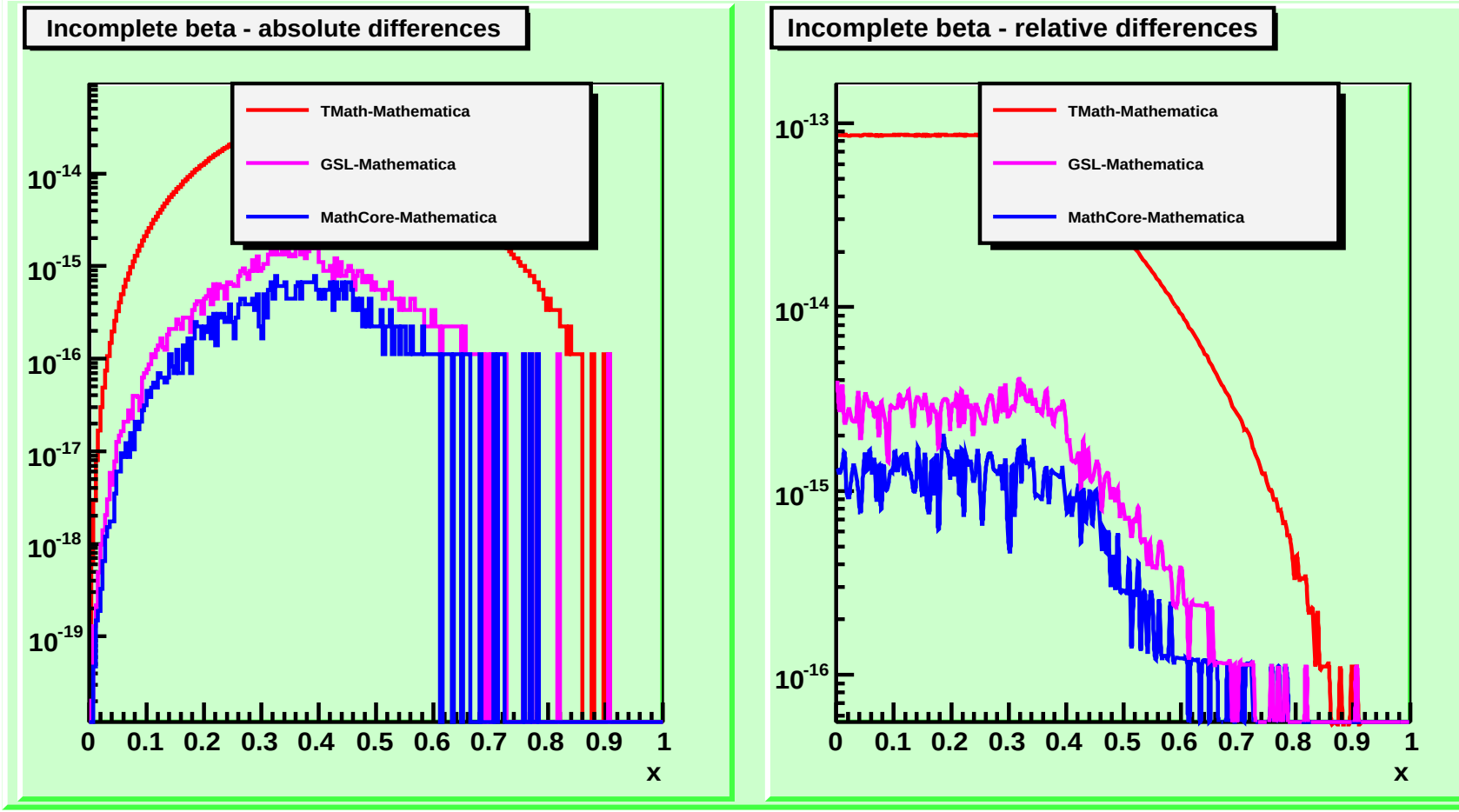


Figure: Comparison with Mathematica BetaRegularized[x,a,b]

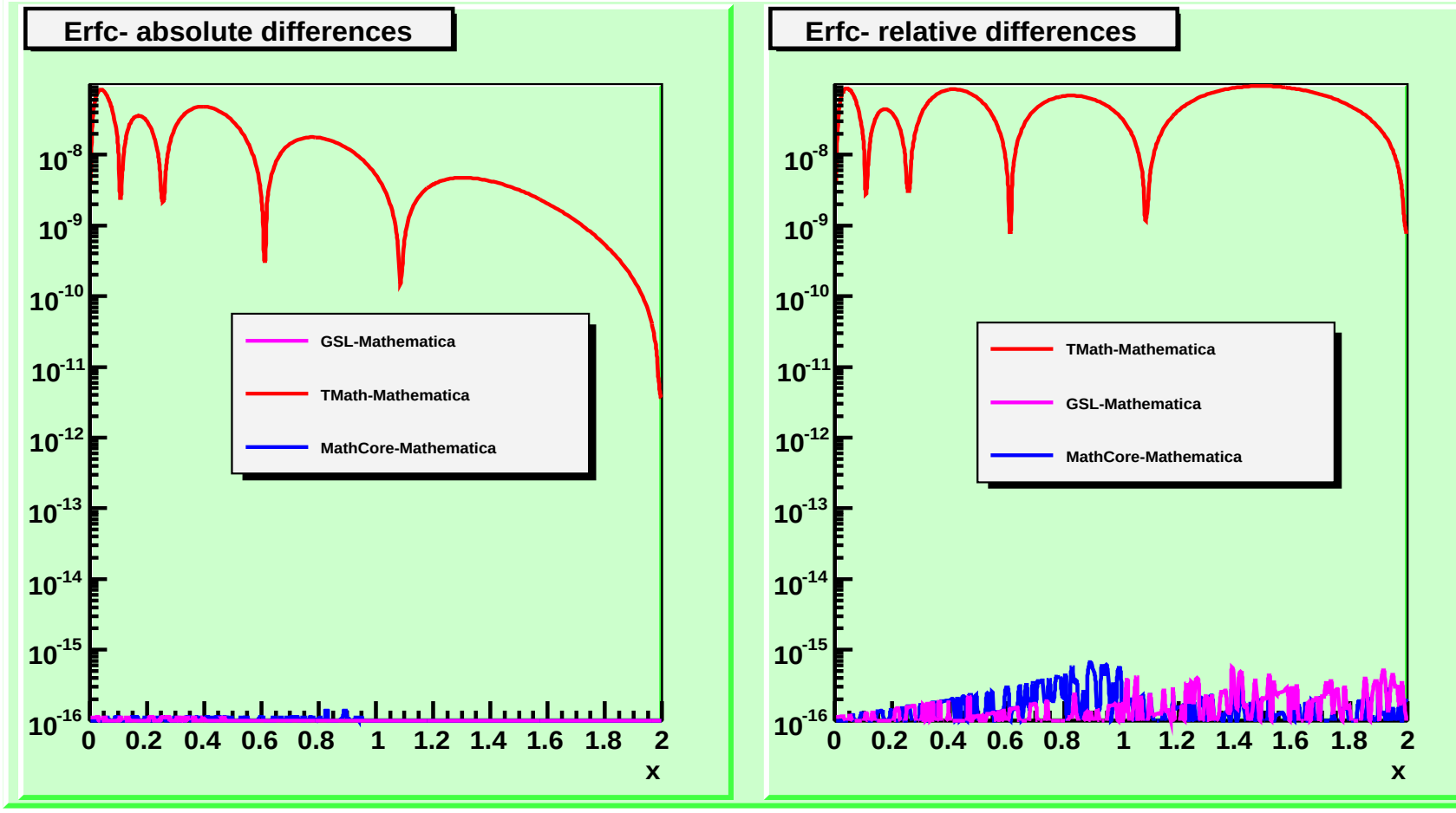


Figure: Comparison with Mathematica Erfc[x]

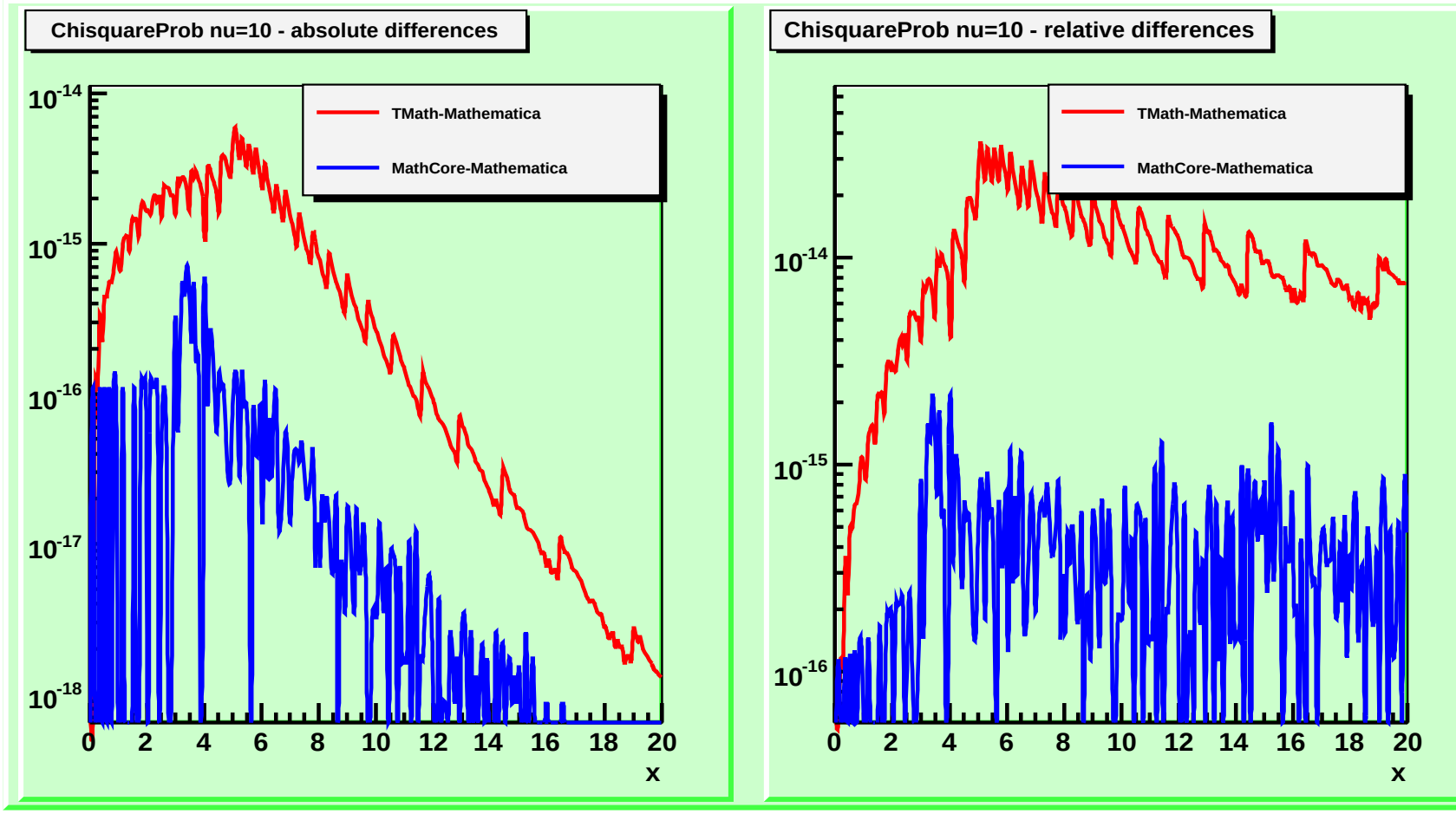


Figure: Comparison with Mathematica ChiSquareDistribution[x]

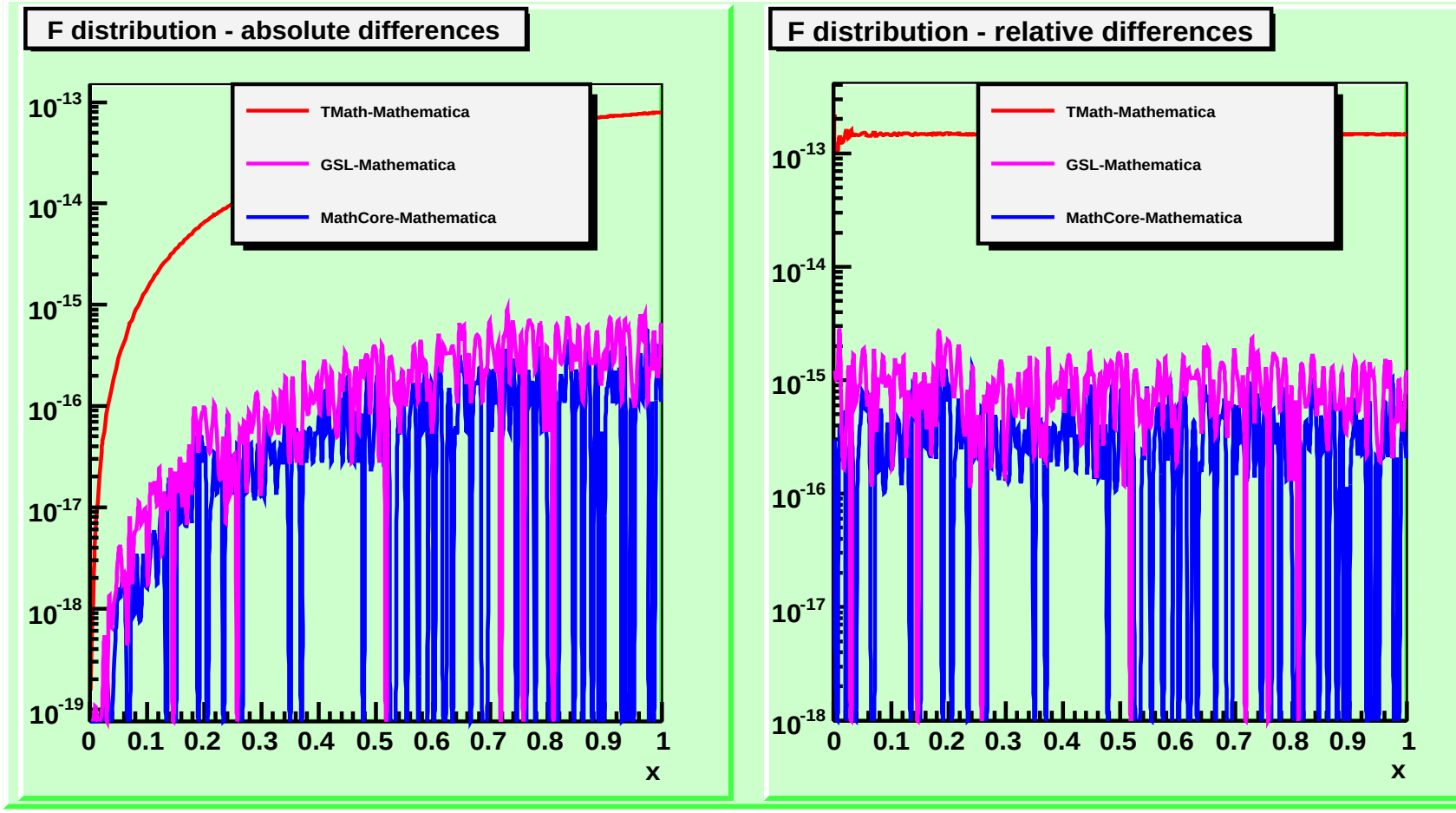


Figure: Comparison with Mathematica FRatioDistribution[x]

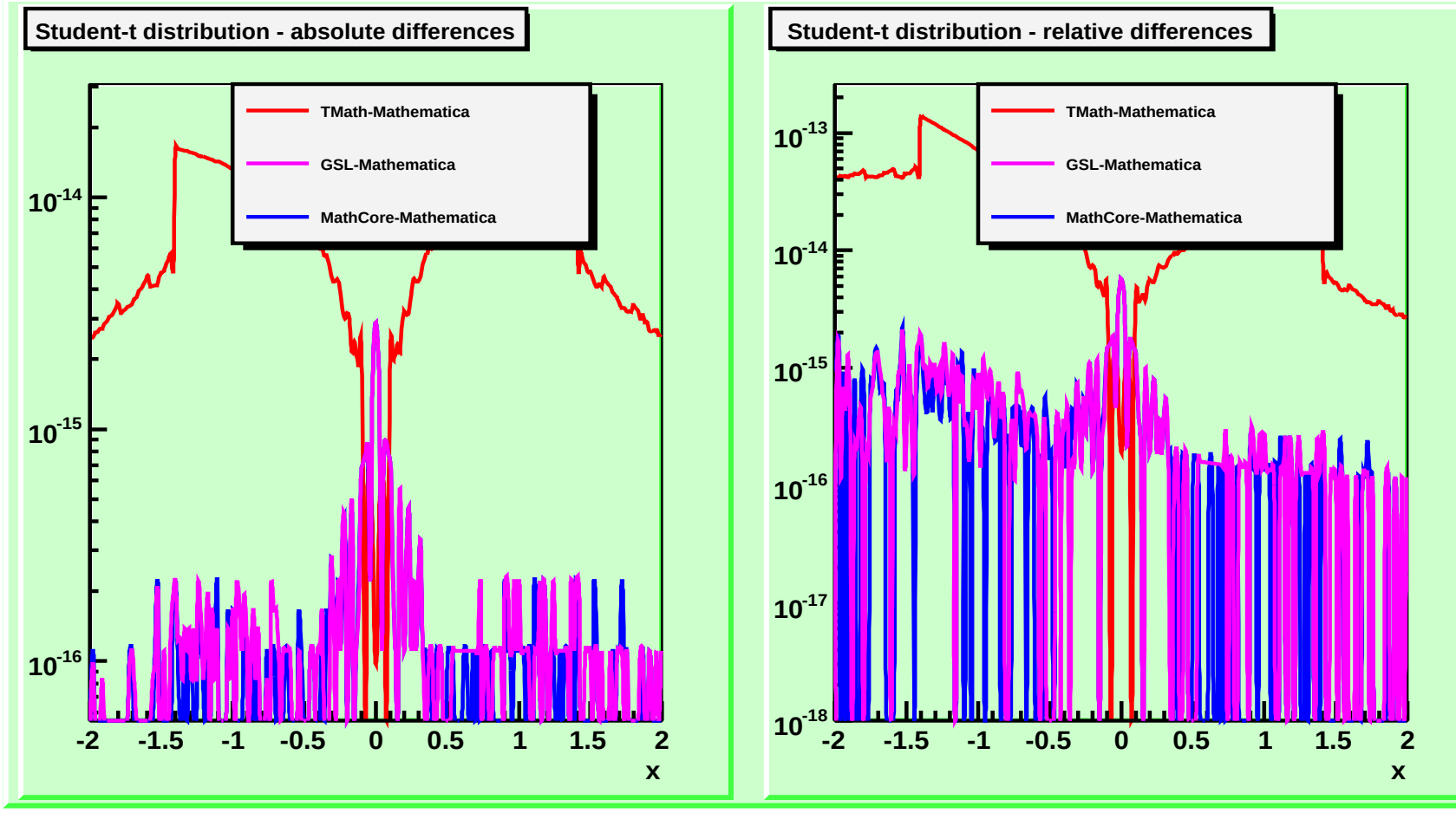


Figure: Comparison with Mathematica