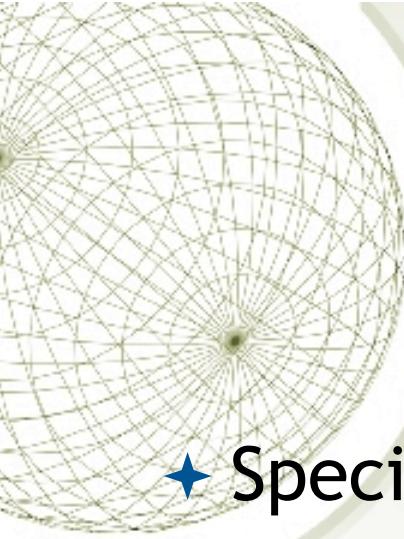


MathMore

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ROOT Workshop 30/9/2005



MathMore components

- ❖ Special functions
- ❖ Statistical functions
- ❖ Generic interfaces
- ❖ Derivation
- ❖ Integration
- ❖ Interpolation
- ❖ Root finding
- ❖ Chebyshev polynomials



The Current Implementation

- ❖ The relevant GSL code extracted into
mathmore/src/gsl-xxx and compiled
automatically
 - ◆ A GSL tar file is in CVS with the extracted code
 - ◆ Works on all supported platforms (thanks to
Bertrand Bellenot for the Windows port)
- ❖ Easily maintainable and updateable
compared to direct copy of the algorithms
into ROOT classes



Special Functions

- ★ Defined in the N1687 Technical Report on Standard Library Extensions
 - ★ <http://www.open-std.org/jtc1/sc22/wg21/docs/papers/2004/n1687.pdf>
- ★ Basic functions in mathcore:
 - ★ Error functions, gamma functions
- ★ The less used and those that use GSL implementation are in mathmore
 - ★ Bessel functions, elliptic integrals, Legendre polynomials etc
- ★ Possibility to migrate functions between mathcore and mathmore transparently for the user



Special Functions cont'd

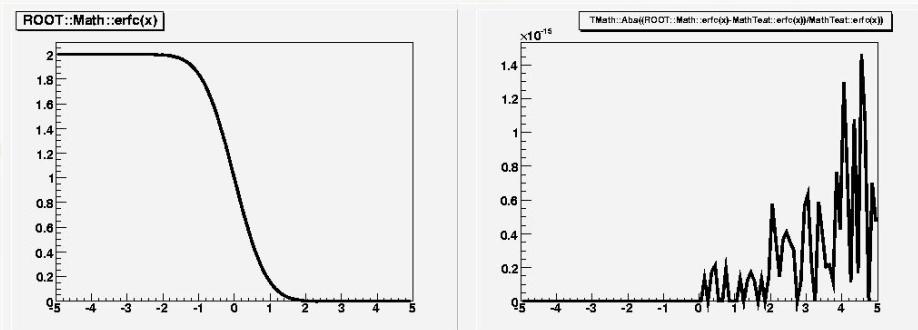
- ❖ Free functions following the C++ standard's naming convention (N1687)
- ❖ Trivial use:

```
root [0] gSystem->Load("libMathMore.so");
root [1] ROOT::Math::cyl_bessel_i(1.2, 2.4)
(double)2.05567401212170076e+00
```

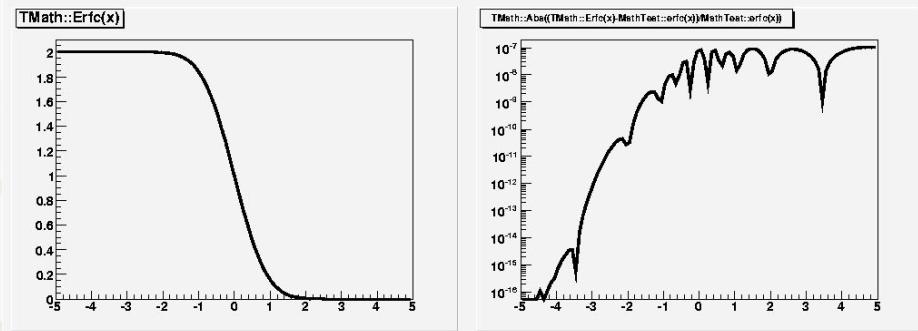
Mathematical Functions tests

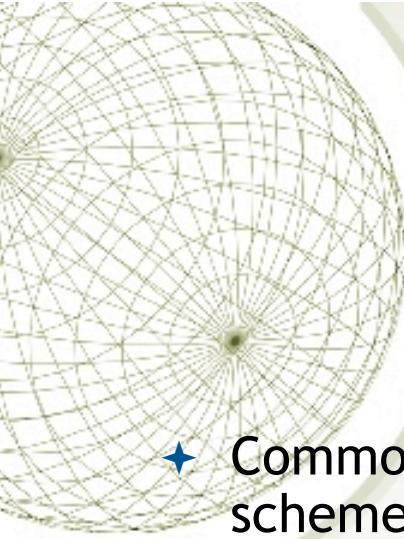
- ❖ New functions improve on the precision of TMath
- ❖ Extensive tests of numerical accuracy, comparisons with other libraries (Mathematica, Nag)

ROOT::Math::erfc and relative difference compared to Mathematica ($\Delta \approx 10^{-15}$)



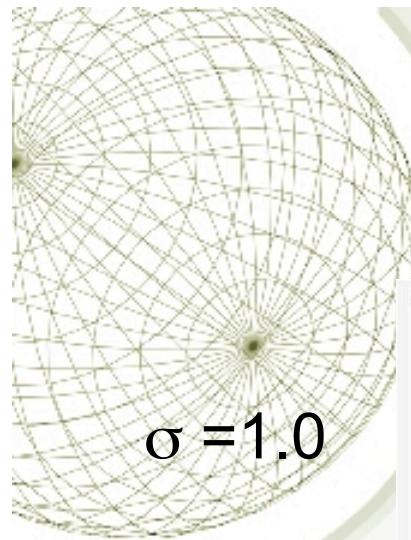
TMath::Erfc and relative difference compared to Mathematica ($\Delta \approx 10^{-7}$)



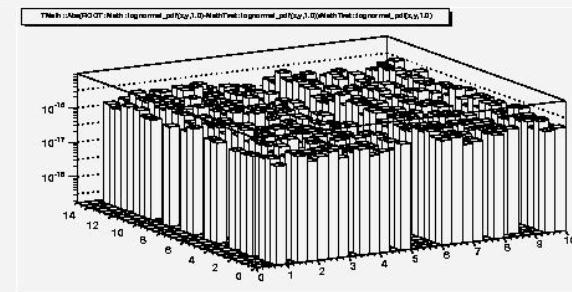
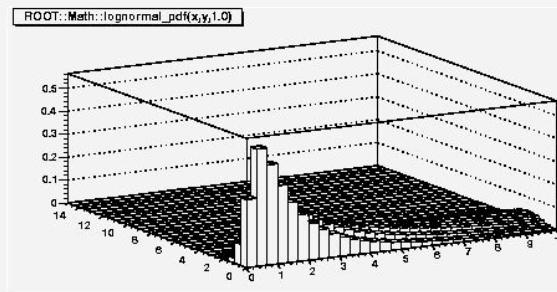


Statistical Functions

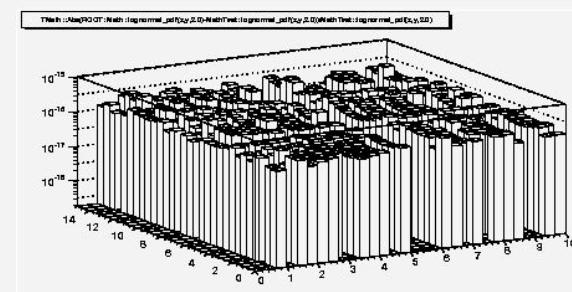
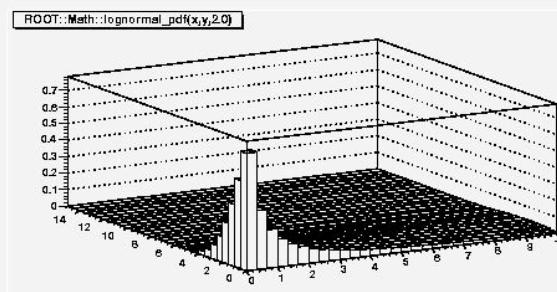
- ◆ Common functions used in statistics with a coherent naming scheme :
 - ◆ Probability density functions (pdf)
 - ◆ Cumulative distributions (lower tail and upper tail)
 - ◆ Inverse of cumulative distributions
- ◆ Examples:
 - ◆ chisquared_pdf
 - ◆ chisquared_prob, chisquared_quant
 - ◆ chisquared_prob_inv, chisquared_quant_inv
- ◆ Naming convention proposed for the C++ standard in N1668, but might change (to be followed closely)
 - ◆ <http://www.open-std.org/jtc1/sc22/wg14/www/docs/n1069.pdf>



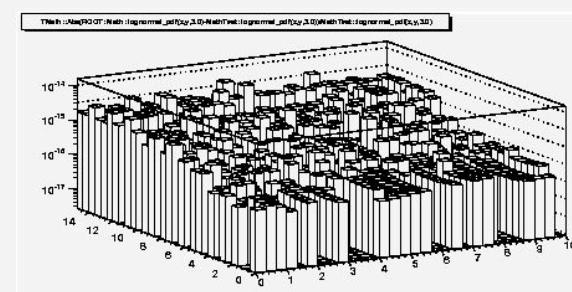
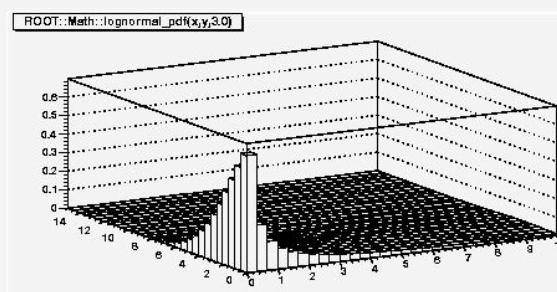
Statistical Functions Tests



$$\Delta \approx 10^{-16}$$

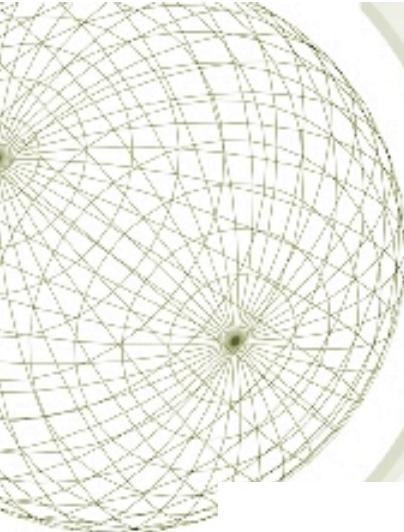


$$\Delta \approx 10^{-16}$$

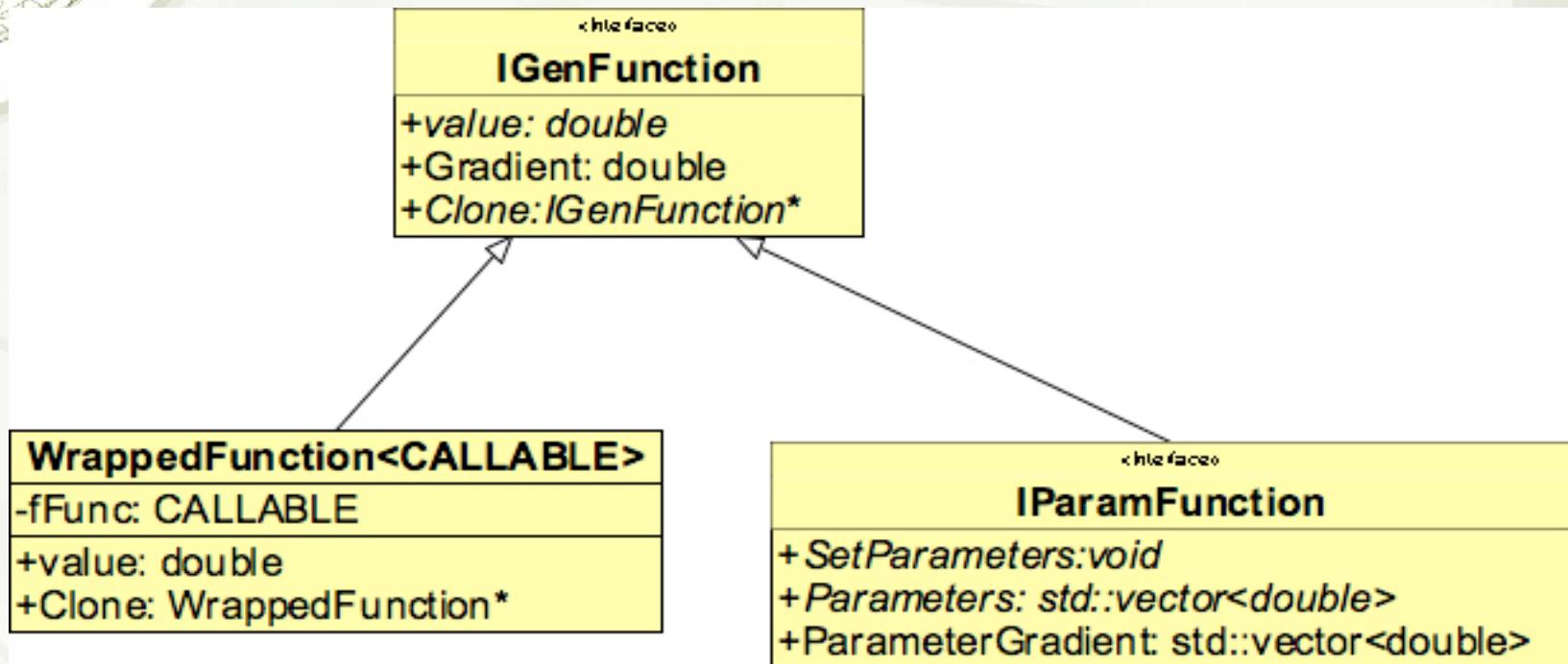


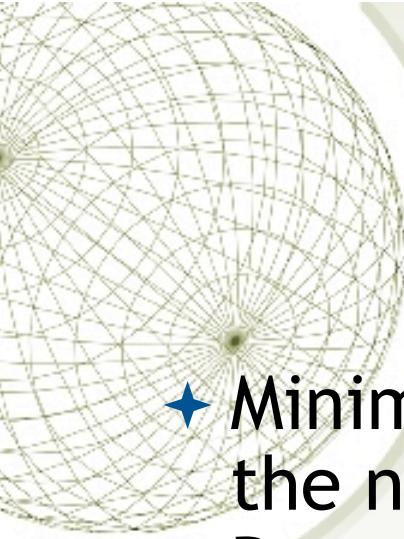
$$\Delta \approx 10^{-16}$$

Lognormal PDF (left) and its Relative Difference Compared to Mathematica (right)



Function Interfaces





Function Interface

- ◆ Minimal interface for functions used by all the numerical algorithms: IGenFunction, ParamFunction, Polynomial (see previous presentations)
- ◆ class WrappedFunction<T> which wraps any C++ callable object (C free functions, functors, etc...)
- ◆ Reviewed by C++ experts – several of the recommendations implemented



Derivation

- ◆ Adaptive central difference algorithm using a 5-point rule
- ◆ Adaptive forward difference algorithm using a 4-point rule
- ◆ Adaptive backward difference algorithm using a 4-point rule



Derivation – an example of the overall design

- ★ Usage with function inheriting from IGenFunction:

```
ROOT::Math::Polynomial *f1 = new ROOT::Math::Polynomial(2);  
...  
ROOT::Math::Derivator *der = new ROOT::Math::Derivator(*f1);  
double x0 = 2;  
double result = der->EvalCentral(x0);  
double error = der->Error();
```

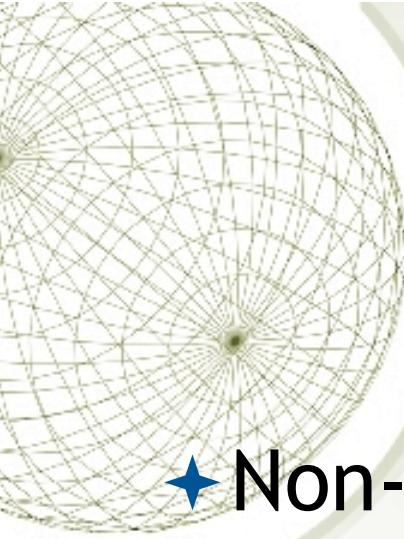


Derivation – an example of the overall design, cont'd

- ★ Usage with a function pointer:

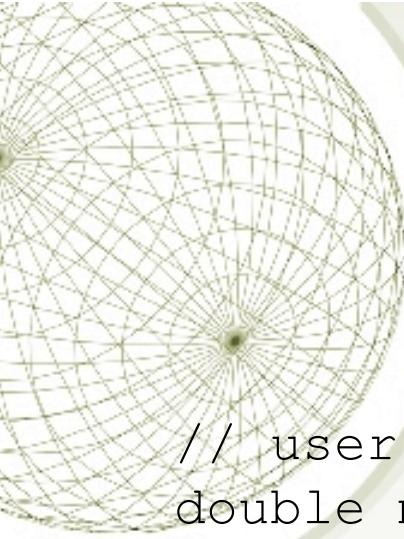
```
double myfunc ( double x, void * ) {  
    return std::pow( x, 1.5 );  
}
```

```
ROOT::Math::Derivator *der = new  
ROOT::Math::Derivator(myfunc);  
double x0 = 2;  
double result = der->EvalCentral(x0);
```



Integration

- ◆ Non-adaptive, adaptive and adaptive singular (i.e. taking into account singularities) integration
- ◆ Different Gauss-Konrod rules can be selected
- ◆ Possibility to use infinite and semi-infinite ranges



Integration Example

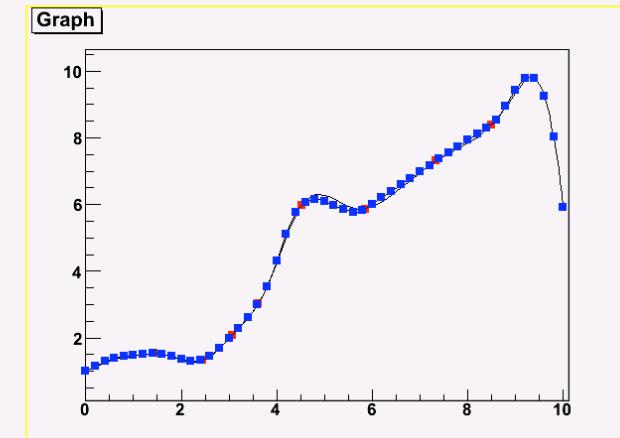
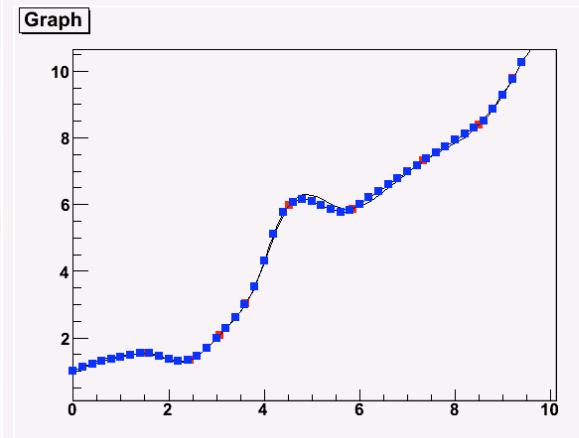
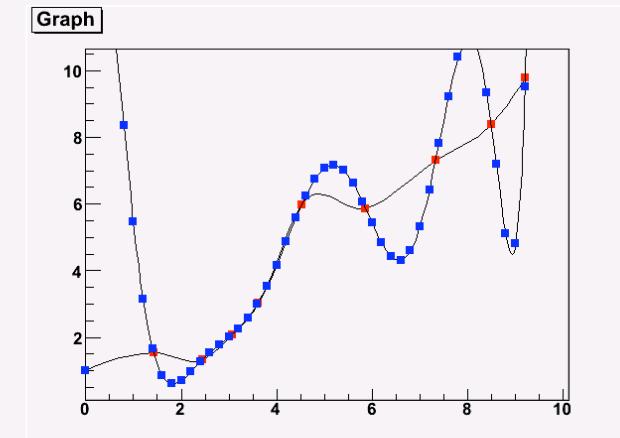
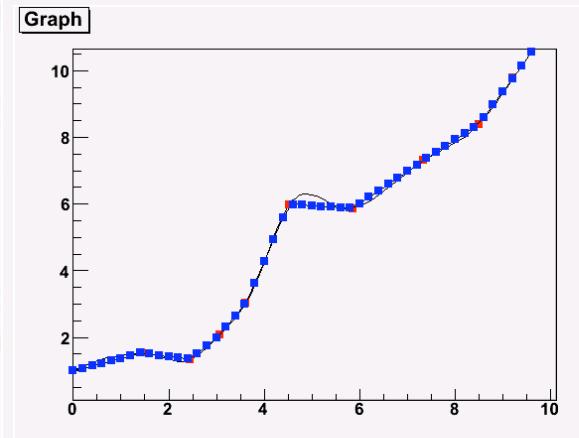
```
// user provided free C function  
double myFunc ( double x) { ... }  
  
// wrap the function  
ROOT::Math::WrappedFunction wFunc(myFunc);  
  
// create integrator and integrate  
ROOT::Math::Integrator ig(wFunc);  
Double result = ig.Integral(a, b);  
Double error = ig.Error();
```

- ❖ **WrappedFunction** can be replaced with any **IGenFunction** in the **Integrator**



Interpolation

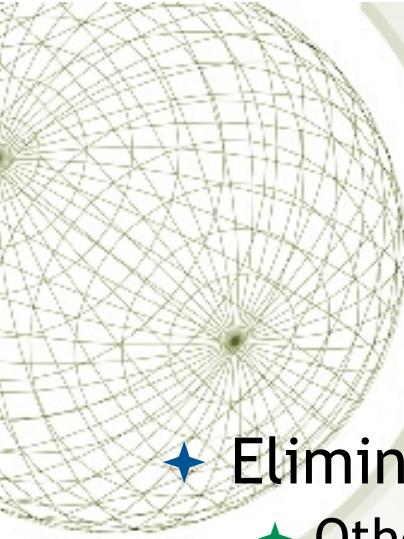
★ Linear,
polynomial,
Akima and
Akima
periodic
interpolations





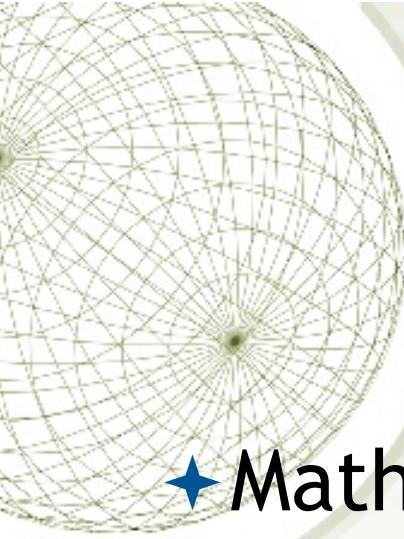
Root Finding

- ◆ Root finding of one dimensional functions
- ◆ Bracketing algorithms: bisection, false position, Brent-Dekker
- ◆ Polishing algorithms (derivatives): Newton, secant, Steffenson



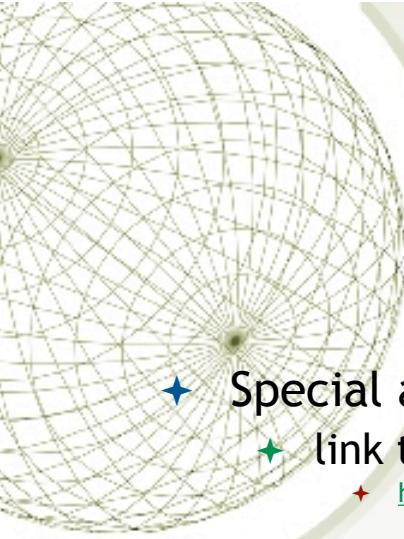
Next Steps

- ❖ Eliminate duplication
 - ❖ Other parts of the ROOT should use mathcore/mathmore
 - ❖ Moving functionality from TMath into mathcore/mathmore
(TMath will remain for backward compatibility)
- ❖ Implement incomplete gamma function in mathcore
(for χ^2)
- ❖ A more detailed discussion is needed to finalize
function interfaces (signatures)
- ❖ Prototype version of TF1 using algorithms from
mathcore and implementing function interface
- ❖ Add algorithms for multi-dimensional functions
- ❖ New additions according to user requests (ex. FFT)



Conclusions

- ◆ Mathmore is available in ROOT 5.04/00 (--enable-mathmore switch in configure)
- ◆ Works on all supported platforms
- ◆ Documentation available at
 - ◆ http://seal.web.cern.ch/seal/MathLibs/MathMore-5_0_4/html/index.html



References

- ◆ Special and Random number C++ extension proposal
 - ◆ link to C++ extension draft
 - ◆ <http://www.open-std.org/jtc1/sc22/wg21/docs/papers/2004/n1687.pdf>
- ◆ Statistical functions proposal to C++ standard
 - ◆ <http://www.open-std.org/jtc1/sc22/wg14/www/docs/n1069.pdf>
- ◆ MathCore reference doc
 - ◆ http://seal.web.cern.ch/seal/MathLibs/MathCore-5_0_4/html
- ◆ MathMore reference doc
 - ◆ http://seal.web.cern.ch/seal/MathLibs/MathMore-5_0_4/html
- ◆ SEAL Math Web site
 - ◆ <http://cern.ch/mathlib>
- ◆ New C++ Minuit Web site
 - ◆ <http://cern.ch/minuit>