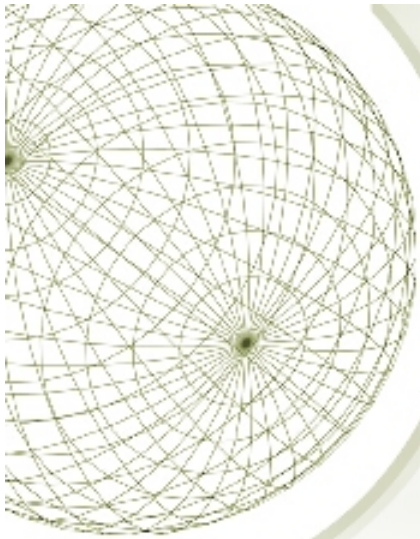


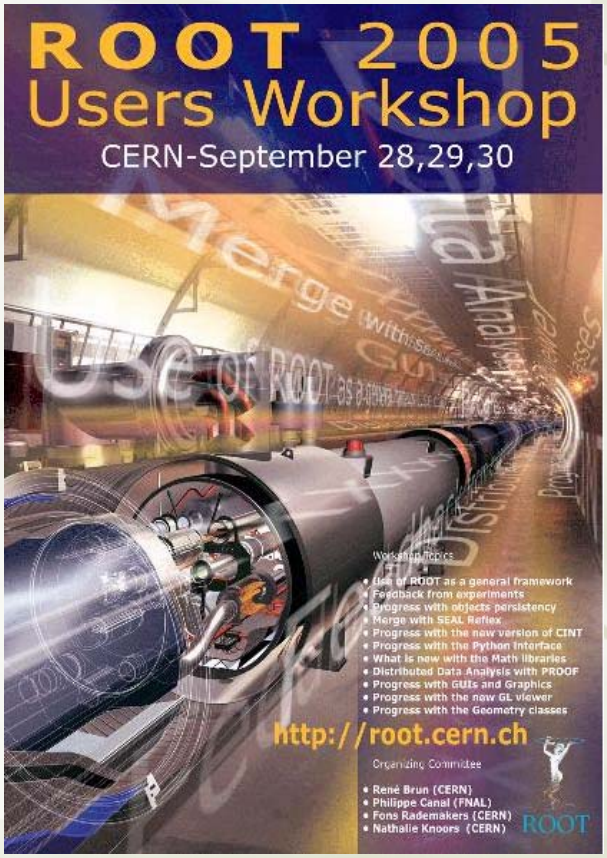
ROOT Math Libraries

ROOT Workshop

30 September 2005

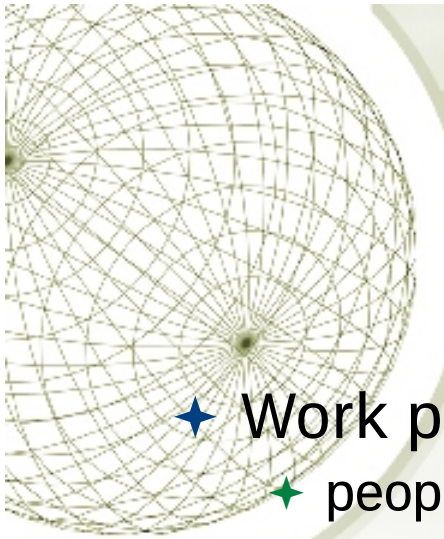
Lorenzo Moneta, Andràs Zsenei

CERN/PH



Outline

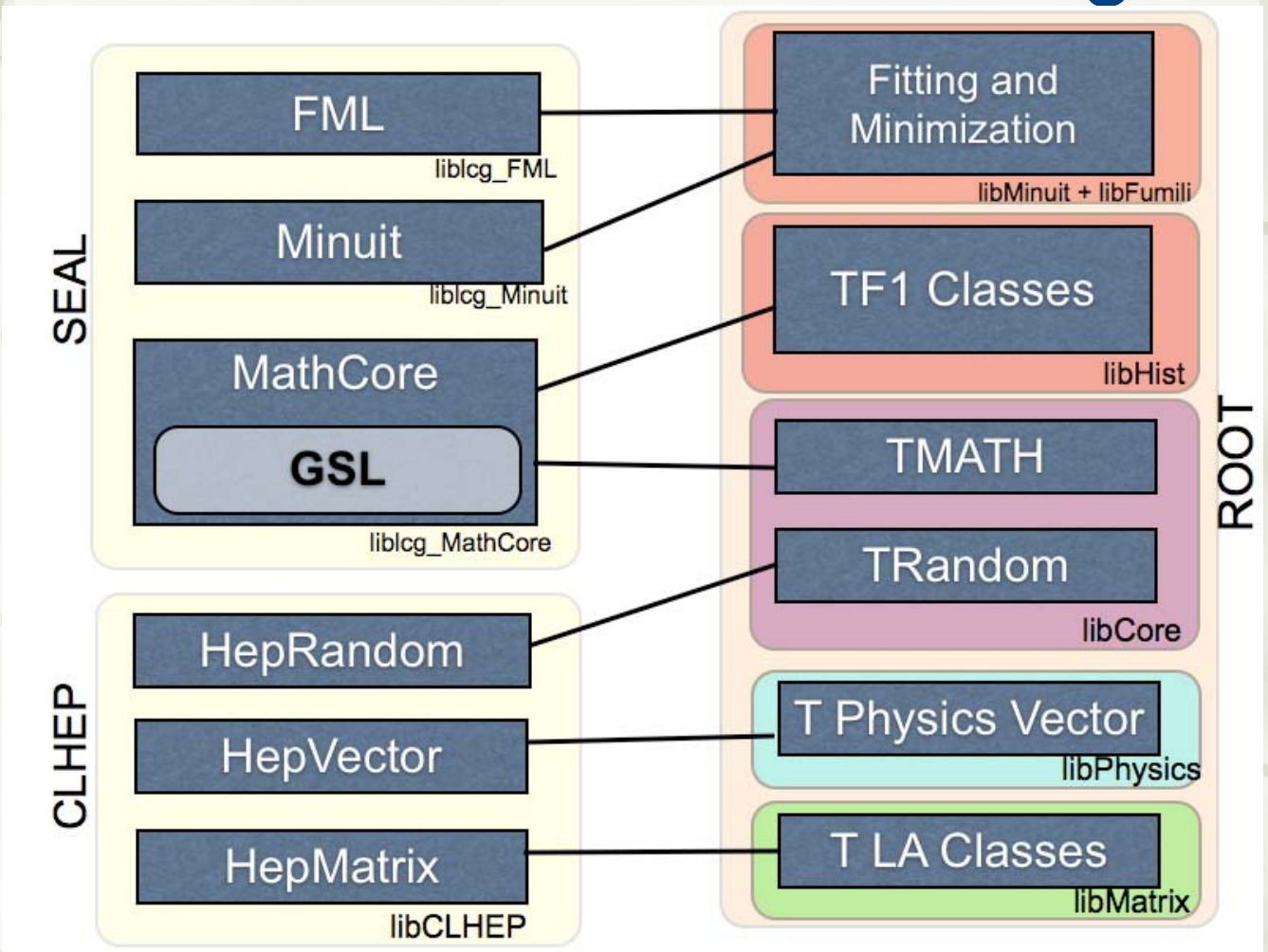
- New ROOT Math libraries
- *Mathcore* contents
- 3D and 4D Vector package
- Future additions to *MathCore*
- Fitting and Minimization
  - New C++ Minuit package



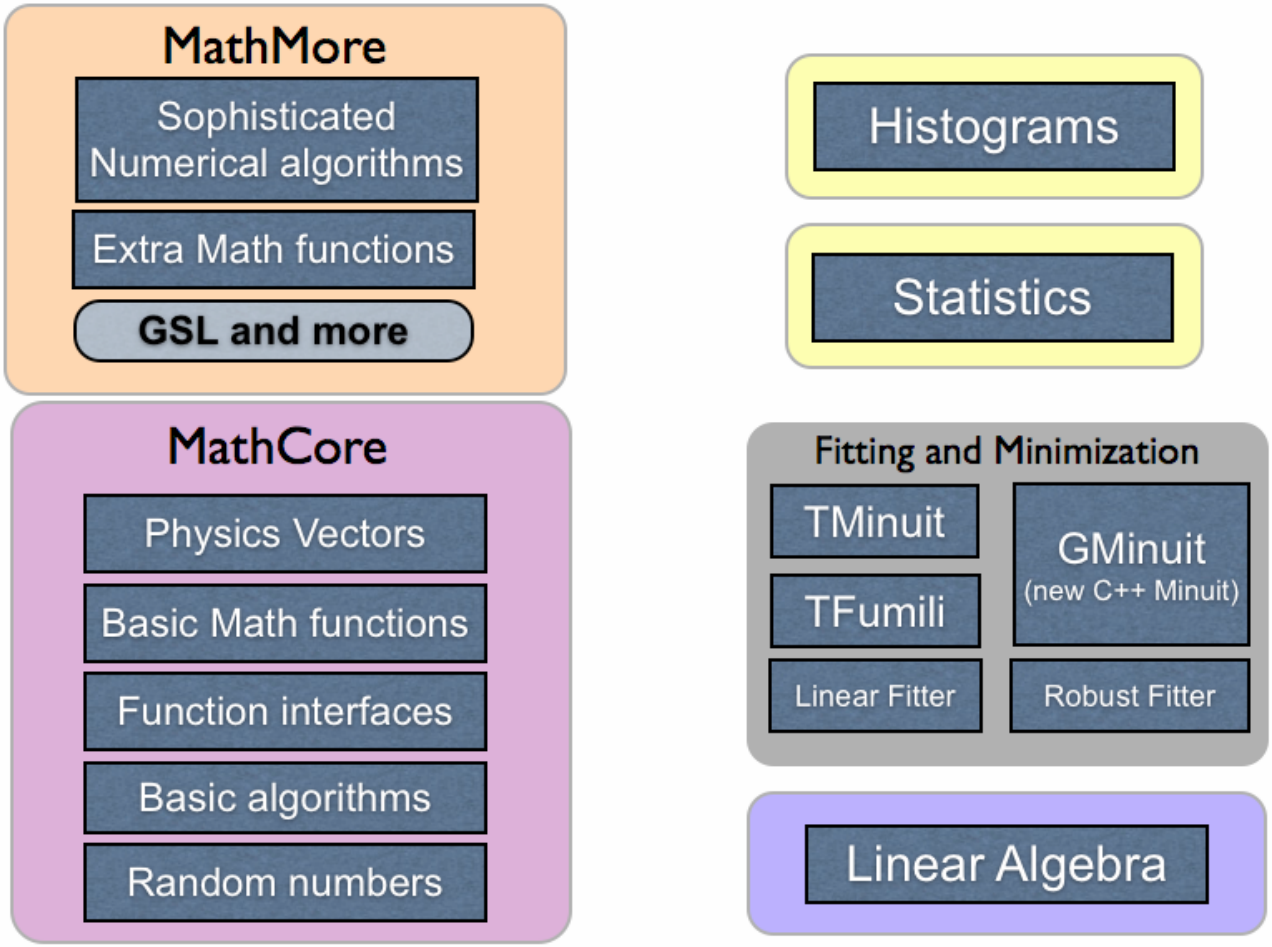
Math Work Package

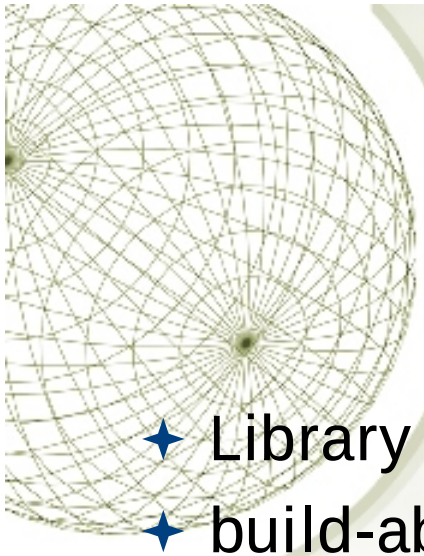
- Work package from ROOT-SEAL merge
  - people: Andras Zsenei, Anna Kreshuk, Lorenzo Moneta, Eddy Offermann
  - contribution also from many other people
    - Walter Brown and Mark Fischler
- Main responsibilities for this work package:
  - Basic Mathematical functions
  - Fitting and Minimization
  - Random Numbers
  - Linear Algebra
  - Physics and geometry Vectors (3D and 4D)
  - Histograms
  - Statistics (confidence levels, multivariate analysis, etc..)

Math Libraries before merge



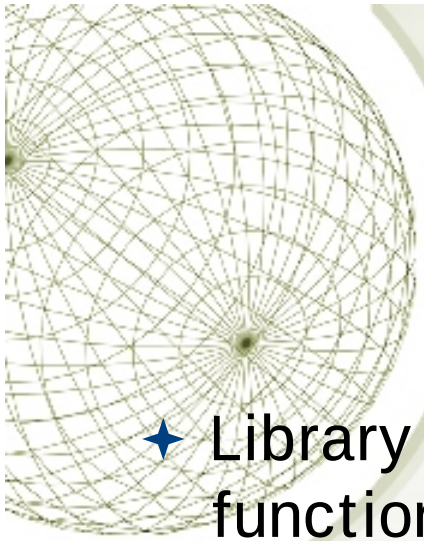
New Math Libraries organization





MathCore

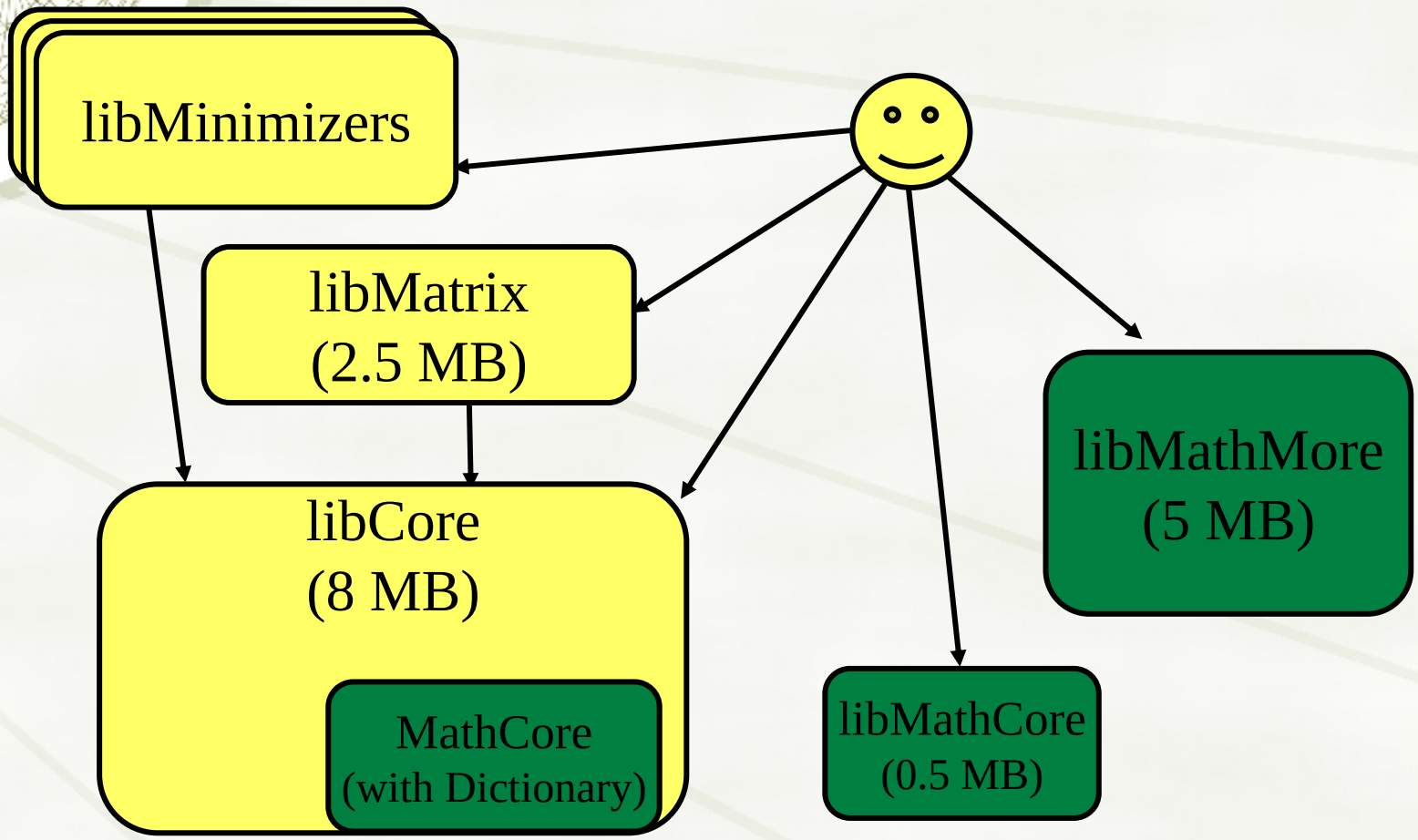
- Library with the basic Math functionality
- build-able as a standalone library
  - no dependency on others ROOT packages
  - no external dependency
- Planned content of *MathCore:*
  - Basic and commonly used mathematical functions
    - Special and statistics (pdf, cdf) functions
      - Implemented using C++ standard extension proposal
  - Interfaces to function and algorithm classes
    - Basic implementation of some numerical algorithms
  - 3D and LorentzVectors
  - Random numbers



MathMore

- Library with more sophisticated mathematical functionalities
- Current content:
  - C++ interface to mathematical functions and numerical algorithms implemented using the Gnu Scientific Library (GSL)
- See next talk (Andras Zsenei)
- repository for needed and useful extra Math functionality
  - could include algorithms extracted from other existing useful math libraries

Library organization



Physics and Geometry Vectors

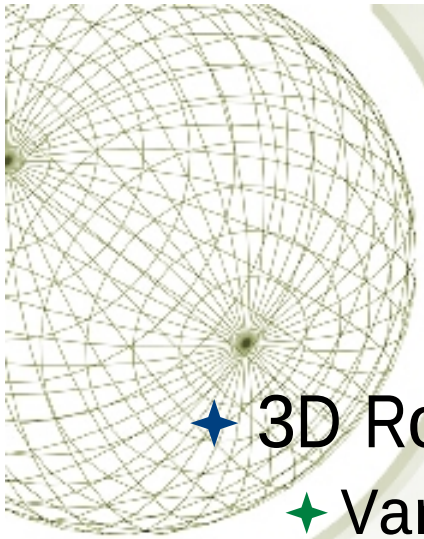
- Classes for 3D Vectors and LorentzVectors with their operations and transformations
  - Merge old ROOT Physics classes and CLHEP Vector and Geometry classes
- Requested by LHC experiments to be used in reconstruction, analysis and in the event data model
- Work done in collaboration with C++ experts from Fermilab computing group
  - M. Fischler and W. Brown
- New classes designed with cleaner and minimal interfaces
  - Try to avoid duplications and aim for stability

New Vector Class Properties

- Vector classes templated on scalar type
- Generalize concept of coordinate systems
  - Vector based on various coordinate system types
    - `LorentzVector<PxPyPzE4D<double> >`
    - `LorentzVector<PtEtaPhiE4D<double> >`
  - Allow conversions and operations between mixed vectors
  - User can choose representation optimal for his use case
  - Use of typedefs to hide template complexity
    - `XYZTVector` for cartesian LorentzVectors
    - `PtEtaPhiEVector` for cylindrical one

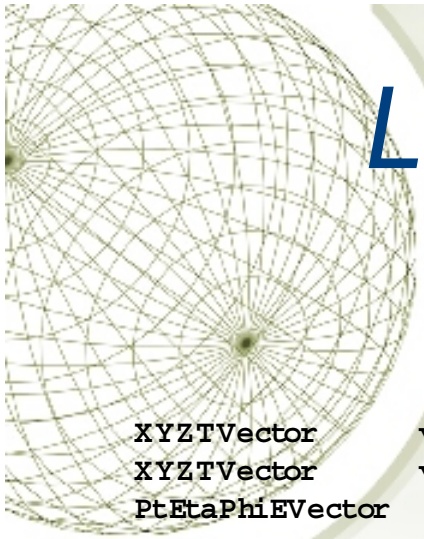
New Vector Class Properties (cont.)

- Points and Vector distinction in 3D
  - Different transformations and operations
    - PositionVector3D class
      - Rotation and translation
      - Cannot be added and difference result is a DisplacementVector
    - DisplacementVector3D class
      - Only rotation (no translation)
      - Have addition and subtraction
  - Describe them as different types
    - not allowed transformations will not compile



Rotations

- 3D Rotations
  - Various classes to describe rotations :
    - 3x3 orthogonal matrix representation
    - 3 Euler angles
    - Direction Axis (Vector) + angle
    - Quaternion (4 numbers)
    - Specialized rotations around X,Y,Z axis
  - Implemented conversions between different types
- LorentzRotation
  - Generic LorentzRotation (4x4 matrix)
  - Boost classes



LorentzVector Example

Constructors

```
XYZTVector       v0;          // create an empty vector (x=y=z=t=0)
XYZTVector       v1(1,2,3,4);    // create a vector (x=1, y=2, z=3, t=4)
PtEtaPhiEVector   v2(1,2,M_PI,5); // create a vector (pt=1,eta=2,phi=PI,E=5)


PtEtaPhiEVector   v3(v1);      // create from a Cartesian4D LV
HepLorentzVector   q(1,2,3,4);    // CLHEP Lorentz Vector
XYZTVector       v3(q)        // create from a CLHEP LV
```

Accessors

```
double x   = v1.X() = v1.Px();       // have both x() and px()
double t   = v1.T() = v1.E();       // have both t() and e()
double eta  = v1.Eta();
XYZVector w = v1.Vec();            // return vector with spatial components
```

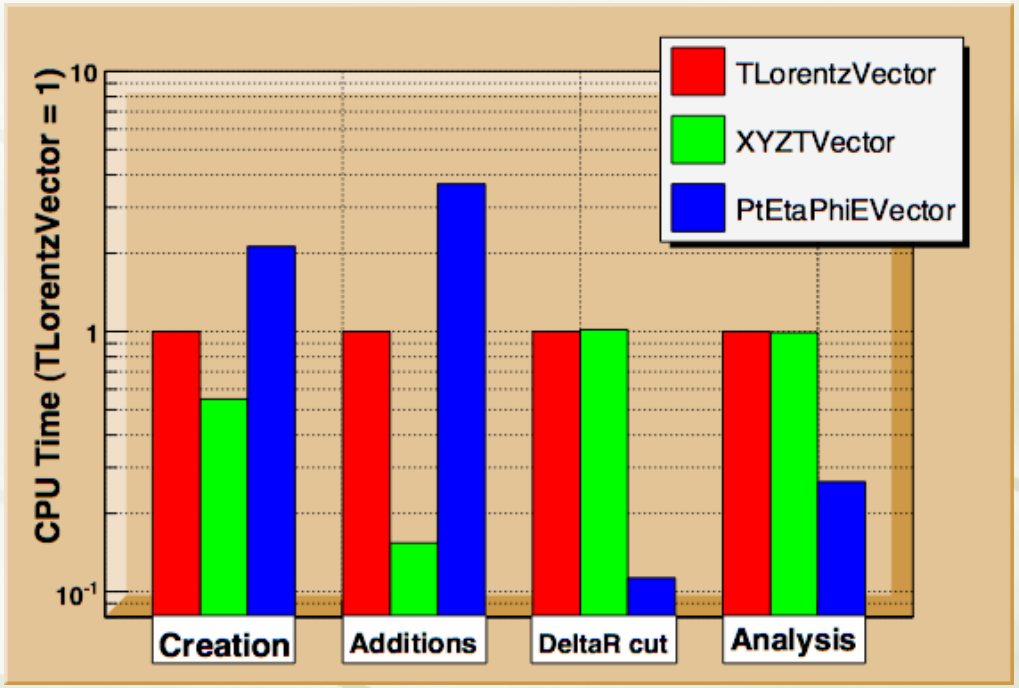
Operations

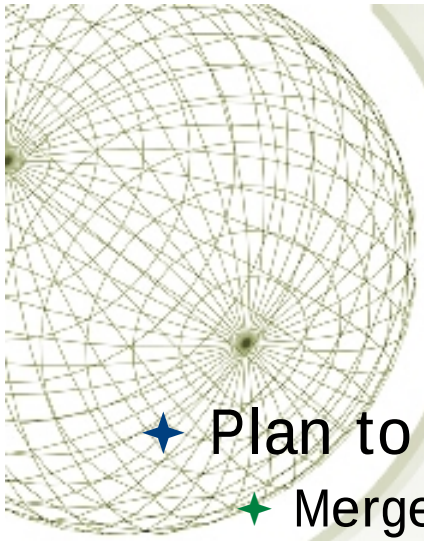
```
v1 += v2; v1 -= v2;              // additions and subtructions
v3 = v1 + v2;
v3 = v1 - v2;
double a; v1 *= a; v1 /= a;         // multipl. and divisions with a scalar
double p = v1.Dot(v2);             // prefer dot (less ambiguous)
```

Vector Performance Tests

- comparison tests with TLorentzVector and also CLHEP
  - performance improvements if used optimal coordinate system
- I/O tests
  - some performance obtained with TLorentzVector if TObject stream is ignored (otherwise performance improvement ~ 20%)

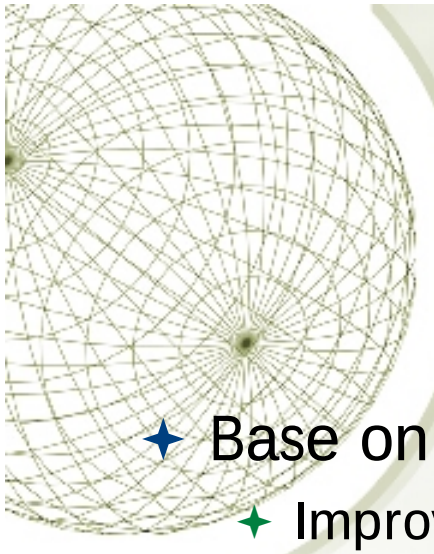
from test program *stressVector* in *root/test*





Random Numbers

- Plan to have as well a new Random number package
  - Merge CLHEP and ROOT Random number classes
  - CLHEP and ROOT have a different design
    - ROOT has a common base class for all the engines and defining also the distributions
      - easier to use (no need to create separate classes)
    - CLHEP separates distribution classes from engine classes
      - easier to extend if user wants to add new distributions
      - distributions classes can have a state
- New design has been proposed to the C++ standard
  - A first implementation is being done by FNAL computing group.
  - We will evaluate it and try to re-implement the TRandom classes using the new library



Linear Algebra

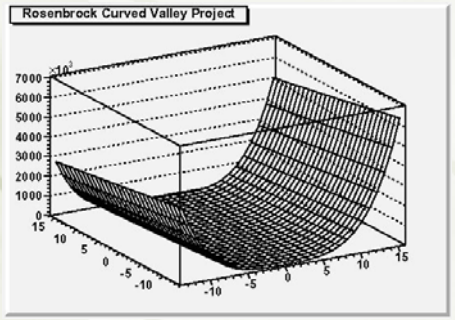
- Base on current ROOT Linear Algebra
  - Improvements are being done to have template matrices
- Continue evaluation tests with other existing packages
  - tvmet, MET, C++ wrappers to BLAS and LAPACK, GLAS (Boost)
- Requests from the experiments for an independent package to replace CLHEP matrices
- Evaluate work needed for producing optimized package for small matrices
  - Typically matrix used in tracking have sizes up to 5
  - Needed only inversions + multiplication
    - No need for full linear algebra functionality

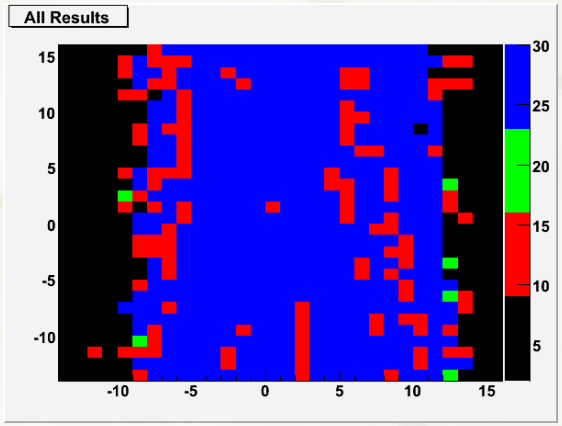
Fitting and Minimization

- A new C++ version of Minuit has been developed within the SEAL project
  - Fortran algorithms have been carefully translated in C++
  - supervised from original author (F. James)
- Same basic functionality as in old version
  - Migrad, Simplex, Minos algorithms
- Extended functionality:
  - Single side parameter limits
  - Added Fumili minimization method for Chi2 and likelihood minimization
- OO package for generic function minimization
  - Easy to extend by inserting new minimization methods

C++ Minuit tests

- Going under extensive performance and convergence tests
  - Same function calls needed to find minimum as in old version
    - Basically the same performance
- Example: test convergence with RosenBrock function





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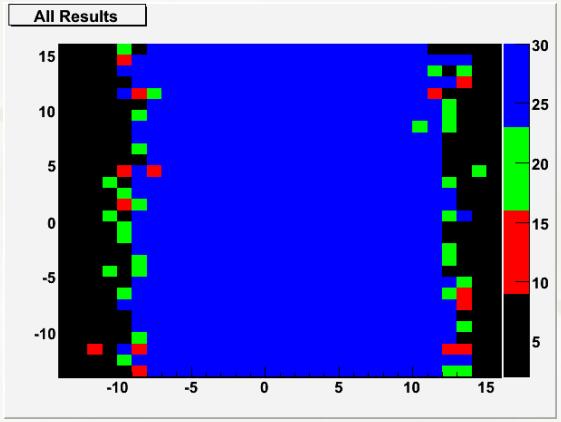
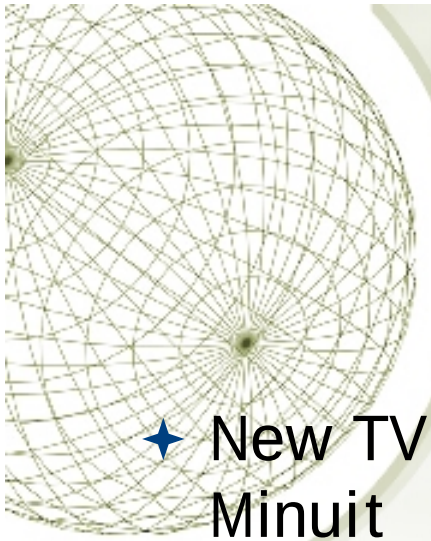
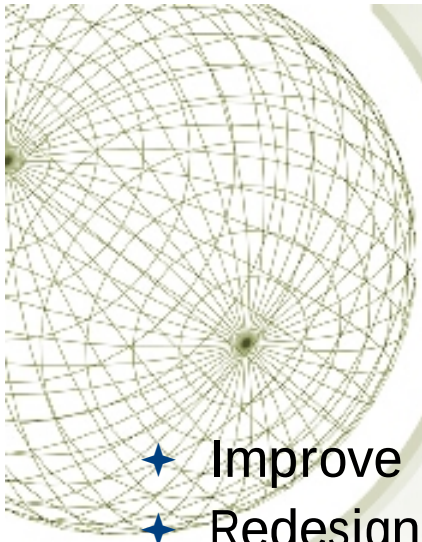


After bug fixes in C++ Minuit



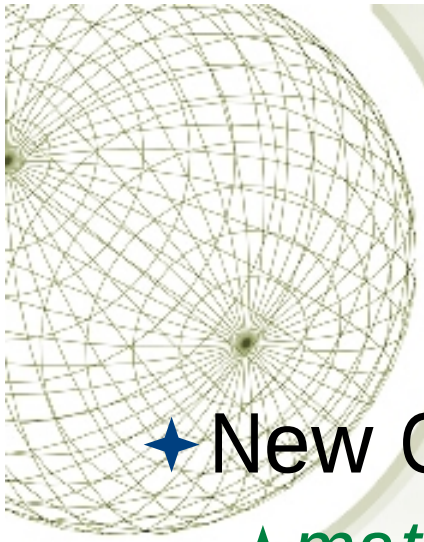
GMinuit

- New TVirtualFitter implementation based on new C++ Minuit
  - GMinuit class
- Performance improvements obtained using an optimized C++ interface
  - Minimization function (FCN) is passed to Minuit as an object
    - Can cache internally its data points used in fitting
    - Can suppress un-used histogram bins (zero entries)
- Plan to add GMinuit in the next ROOT release
- Implement a backward-compatible interface for new C++ Minuit



Plans for New Fitter interfaces

- Improve fitting and minimization interface in ROOT
- Redesign taking into account all fitter and minimizer methods present in ROOT
  - Linear and robust fitter, fraction fitter
  - Minuit (Migrad, Simplex), quadratic optimization
  - RooFit
- Idea is to have separate interfaces:
  - Fitting interfaces used to construct an objective function (chi2, likelihood) from data and model function (pdf)
  - Minimization interfaces to perform the task of finding the function minimum
    - Various minimizers implementations as separate plug-ins
- Use common function interfaces defined in *MathCore* for numerical algorithms

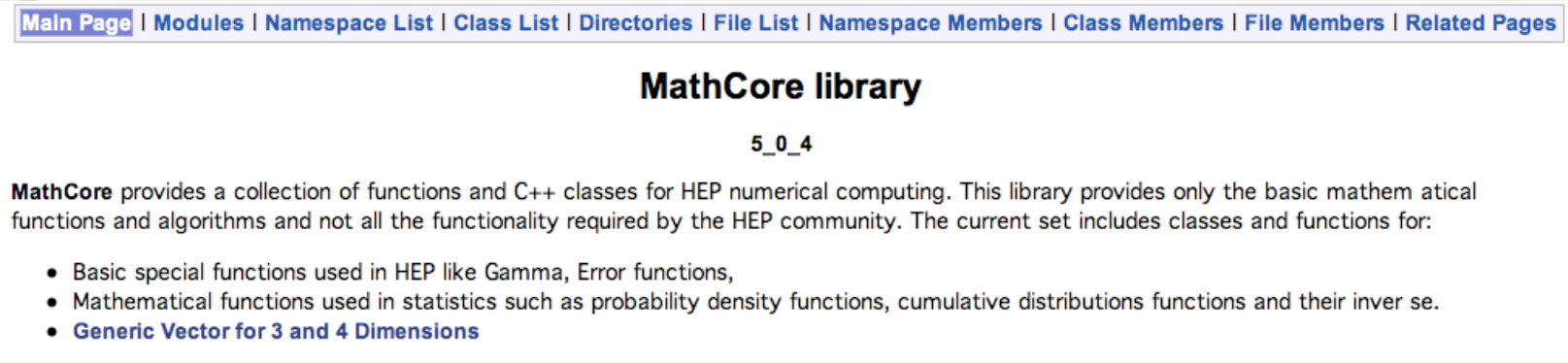


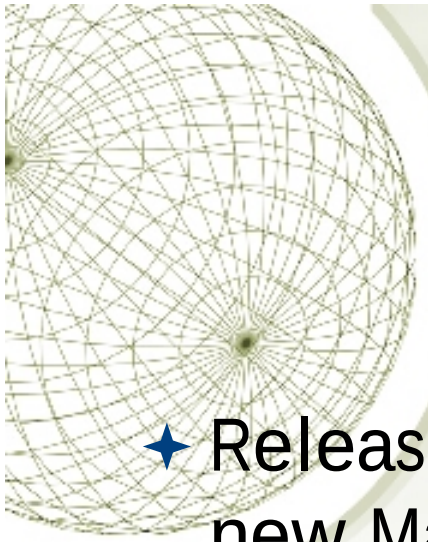
Integration in ROOT

- New CVS directory existing in ROOT 5
  - *mathcore* and *mathmore*
  - Build now as separate library *libMathCore* and *libMathMore*
    - plan is to have *MathCore* in *libCore*
- Classes are in namespace *ROOT::Math*
- Public header files are in *include/Math*
  - Possible transparent transition of classes *MathCore* ⌦ *MathMore*

MathCore Current Status

- Available now in *MathCore*:
  - 3D and 4D Vector package
  - basic Math functions
- Can be downloaded as a tar file and built independently from other ROOT libraries
- Documentation available at
  - http://seal.web.cern.ch/seal/MathLibs/MathCore-5_0_4/html/index.html





Conclusions

- Released since June (ROOT) first version of new Math library (*MathCore*)
- *MathMore* is available in 5.04 (see next talk)
- Future work:
  - Add Random numbers
  - Define interfaces for functions and numerical algorithms to be used by client libraries (TF1)
  - Redesign fitting interfaces
  - Import new C++ Minuit