

Final Report of the RTAG on Mathematical Libraries

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2 The mandate:

- Review the current situation of the usage of the various math libraries in the experiments (including, but not limited to, Nag-C, GSL, CLHEP, ROOT)
- Identify and recommend which ones should be adopted, which ones could be discontinued
- Suggest possible improvements to the existing ones
- Estimate resources needed for this activity

3 Assessment of present situation

Mathematical libraries can be classified in three categories:

1. **Libraries developed within the HEP community:** We have considered CLHEP, ZOOM, ROOT. These libraries are expected to be available also in the future and to evolve to meet future needs; however, as the resources are limited, they cannot cover the general mathematical functionality.

2. **Special-purpose libraries** optimized for basic operations on data types like matrices. We have considered Blitz++, Boost, TNT, MTL. These packages usually concentrate on a specific topic and use modern OO methodologies and techniques for their design and implementations. Other packages are expected to appear on the market in the future, therefore a regular assessment of the situation is recommended.
3. **General purpose mathematical libraries.** We have considered NAG-C and GNU Scientific Library (GSL).

Presently, all of these libraries are used in the experiments, in addition also Fortran libraries (CERNLIB) and Fortran programs (automatically) converted to C. This is expected to evolve quickly to the use of pure C++ libraries in most experiments, but still the basic lesson is that physicists will use whatever is available. They don't have time to seek common solutions even within an experiment and certainly not between experiments.

4 Financial Considerations

4.1 License Fees

All libraries considered are available at little or no cost as source code under an OpenSource license, except NAG-C.

4.2 NAG-C

The NAG-C library is of very high quality and we expect to have this available (with a site-license) at all major institutions, i.e., Tier-0 and 1 centres. However, for use outside these centres, LHC-wide developer licenses are needed. The additional cost is estimated at about 300 kCHF per yr initially, and would drop to less than 100 kCHF per yr for the maintenance period after about 4-5 years. This is a rough estimate, since a new improved and more expensive release is expected soon, and all this is anyway subject to negotiation. A major decision will have to be made as to whether this library will be needed (and therefore the additional cost will have to be paid) or whether development can be done using another (free) library. This decision can be made only after the study proposed in Recommendation 3 below.

4.3 GNU Scientific Library

The GNU Scientific Library (GSL) has been identified as the best candidate to replace the NAG-C library as it is also a generic mathematical library with a very rich set of functionality. The comparative evaluation of GSL and the NAG-C is a big job which will require not only extensive testing, it must be done by experts who understand the numerical and mathematical aspects involved.

4.4 General Support

In addition to license fees (NAG only), it must be remembered that any package (including free software) requires resources to make it available conveniently and to see that it is used intelligently. This means at least one librarian, a webmaster and several people providing expertise in mathematical methods and numerical and statistical analysis.

5 Recommendations

1. A support group should be designated to provide advice and information about the use of existing libraries, to assure their continued availability, to identify where new functionality is needed, and to develop that functionality themselves or by coordinating with other HEP-specific library developers. This group could be a new group set up at CERN in order to be as close as possible to the experiments, but it could also be one of the existing software groups at CERN or another major lab, or possibly a collaboration between two or more such groups. The goal would be to have close contact with the experiments and provide expertise on mathematical methods, aiming at common solutions.
2. The experiments should maintain a data base of mathematical libraries used in their software, and within each library, the individual modules used. This is in their own interest, since only in this way can continued support for these libraries be guaranteed.
3. A detailed study should be undertaken to determine whether there is any functionality needed by the experiments and available in the NAG library which is not covered as well by a free library such as GSL. This is a big job which could be done by an outside group such as the Centre for Advanced Technology, Indore, India which has recently entered into an agreement with CERN for providing a major software contribution. The interface with the experiments would be assured by the support group mentioned above.