

The Biochemical Algorithms Library (BALL) - Rapid Application Development in Structural Bioinformatics

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Developing programs for structural bioinformatics is a difficult and often tedious task. Even if the algorithms have been carefully designed, the programmer has to solve a variety of complex and recurring problems not fundamentally related to the algorithm at hand, but necessary for real-world applications.

With the Biochemical Algorithms Library (BALL), we present a versatile C++ class library for structural bioinformatics that is supplemented with a Python interface for scripting functionality and a number of applications like the molecular modeler BALLView.

In recent years, BALL has seen a significant increase in functionality and substantial useability improvements. It has been ported to further operating systems; indeed, it currently supports all major brands. Moreover, BALL has evolved from a commercial product into a free-of-charge, open source software licensed under the Lesser GNU Public License (LGPL).

The current version (1.3.2 at the time of writing) contains more than 730 classes and more than 700,000 lines of code. Of these, we want to briefly highlight some of BALL's most important features and will show some ways in which the use of such an rapid application development framework can simplify the life of scientists and developers.