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BzzMath library upgrading

WARNING

Some portions of the tutorial and of the same BzzMath library are in progress for upgrading, extension, and revision.

For any problem you may encounter using the BzzMath library please contact the Author at: guido.buzziferraris@polimi.it

Users are kindly pleased to point out any kind of bug or problem in general to fix them.

BzzMath is constantly upgraded. You can find the last version at:

www.chem.polimi.it/homes/gbuzzi
BzzMath library requirements

WARNING


According to the compiler, some additional operations must be accomplished as described in the following.

If you want to use the BzzMath tutorial, you will need PC with Microsoft Power Point 2003 or higher.
You have to perform the following general task

Unzip the file BzzMath7.zip in one directory (for example in the C: root) present in your PC. This directory will be called DIRECTORY.

This unzip makes the following task.

A. The subdirectory BzzMath is created into the directory DIRECTORY

B. Five subdirectories named lib, hpp, exe, Examples and BzzMathTutorial are created into DIRECTORY\BzzMath directory

C. The BzzMath.lib library is copied into DIRECTORY\BzzMath\Lib subdirectories, according to the selected compiler one would use

D. All of the .hpp files are copied into DIRECTORY\BzzMath\hpp directory

E. All of the .exe files are copied into the DIRECTORY\BzzMath\exe directory

F. All of the tutorial .ppt files are copied into the DIRECTORY\BzzMath\BzzMathTutorial directory

G. All of the examples files are copied into the DIRECTORY\BzzMath\Examples directory
1. In Microsoft Developer Studio 6.0 or later, open Options in the Tools menu option, then choose the Directories tab and add the directory specification DIRECTORY\BzzMath\hpp for include files.

2. Add DIRECTORY\BzzMath\exe and DIRECTORY\BzzMath\BzzMathTutorial in your operating system (Windows) PATH option: Click with the right mouse button on System Resources. Choose the Properties option. Choose the Advanced option. Choose Environment Variables. Choose the PATH option. Add the voice:

;DIRECTORY\BzzMath\exe; DIRECTORY\BzzMath\BzzMathTutorial;

Please note that when you add a new directory to the PATH environment variable you MUST add a “;” character (without quotes) before specifying the new directory.

After having changed the PATH Environment Variable you must restart the computer.
A. Visual C++ 6.0 (32 bit)

The proper library (DIRECTORY\BzzMath\Lib\VCPP6\BzzMath.lib) must be added to the project. No additional operations must be accomplished using VC++ 6.0.

The program must start with the following two statements:

#define BZZ_COMPILER 0 // optional (default value)
#include “BzzMath.hpp”

B. Visual C++ 2008 (32 bit)

Users adopting VC++ 2008, must use the proper library (DIRECTORY\BzzMath\Lib\VC2008\BzzMath.lib) and replace the default (DLL) run-time library. Select:

    Project/ Properties/ Configuration Properties/ C/ C++/
    Code Generation/ Runtime Library

There, if one is working in Release, the Multi-threaded (/MT) library must be selected; in Debug the Multi-threaded Debug (/MTd) must be selected.

The program must start with the following two statements:

#define BZZ_COMPILER 1
#include “BzzMath.hpp”
Use of BzzMath library 7.1

C. Intel 14.0 (64 bit)

Users adopting this compiler must follow what described at the point B. using the proper library (DIRECTORY\BzzMath\Lib\INTEL_WINDOWS\BzzMath.lib).

The program must start with the following two statements:

#define BZZ_COMPILER 11
#include "BzzMath.hpp"

D. Visual C++ 2010, 2013 (64 bit)

Users adopting VC++ 2010 and 2013, must use the proper library (DIRECTORY\BzzMath\Lib\VCPPxx\BzzMath.lib), where xx=2010 for 2010 and xx=2013 for 2013, and replace the default (DLL) run-time library. Select:

Project/ Properties/ Configuration Properties/ C/ C++/
Code Generation/ Runtime Library

There, if one is working in Release, the Multi-threaded (/MT) library must be selected; in Debug the Multi-threaded Debug (/MTd) must be selected.

The program must start with the following statements:

#define BZZ_COMPILER 2 //for C++ 2010
//#define BZZ_COMPILER 3 //for C++ 2013
#include “BzzMath.hpp”
Linux users have to develop their own makefile including the appropriate .hpp and .lib PATHS for each project. Also the proper library has to be selected:

**Compiler gcc:**

```
DIRECTORY\BzzMath\Lib\Linuxgcc\BzzMath7.a
```

The program must start with the following two statements:

```
#define BZZ_COMPILER 101
#include "BzzMath.hpp"
```
openMP Windows compatibility

A. Visual C++ 6 users

No parallel computing is allowed in BzzMath library 7.


People using these compilers must activate openMP library option for exploiting parallel computing with BzzMath library 7.1.

Select:

Project/ Properties/ Configuration Properties/ C/ C++/ Language
and activate openMP Support.
Manage openMP during computations

BzzMath library uses openMP directives for parallel computing by default when the compiler support them.

The user who wants to personally manage openMP library must deactivate the parallel computing within the BzzMath library to prevent any kind of parallel computing overlapping.

Inside the main, the first statement must be:

```
bzzOpenMP = 0;
```
Then you can start using the **BzzMathTutorial.pps** file in the **DIRECTORY\BzzMath\BzzMathTutorial** directory


Changes from BzzMath 5 to 6

There is a single library **BzzMath.lib** and single header file **BzzMath.hpp**

All the classes and functions belonging to **BzzMath 6.0** use double precision by default (i.e., **BzzVectorDouble** is now **BzzVector**)

Single precision is not available anymore

Factored becomes Factorized in classes and functions belonging to **BzzMath** (i.e., **BzzFactoredLQ** is now **BzzFactorizedLQ**)

Numerical improvements were introduced in many classes. In addition, new classes were added to.

Besides VC++ 6.0, compatibility was extended to: VC++ 7.0, VC++ 8.0, and VC++ 9.0 with openMP 3.0; Intel 11.0 with openMP 3.0; and Linux Intel 11.0 and Linux g++ with openMP.
Changes from BzzMath 6 to 7.1

Numerical improvements were introduced in many classes. In addition, new classes were added to (see references).

Compatibility of BzzMath 6.0 has been extended in 7.1 to: VC++ 2010 and VC++ 2013 with 64 bit and INTEL 14.0.


BzzMath 7.1 is now available for Linux compiler gcc.