Polytopal Cell Complex (PCC) Processing Design (CPD code\*)

Technical Manual

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**The code online source repository:** <https://github.com/PRISBteam/PCC_Processing_Design>

**The code reference example:**

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CPD code is fully written in C++ as a CMake project (can be launched using CMakeLists.txt file) and consists of several modules-libraries, configuration < \*.ini> files governing the code execution, sources of PCCs as discrete combinatorial spaces, and databases of material parameters. For successful code execution, both the C++ compiler and CMake software must be installed. The code is tested for C++17 and works well with CMake 3.23 , g++ compiler and CLion IDE. The code uses explicitly the Eigen and Spectra libraries which must be downloaded (from <https://spectralib.org/download.html>) and copied to the directory containing all the STL C++ libraries on the local PC. The code works with a pre-created PCC (please see more details on the <http://materia.team/> project page) represented in the form of incidence and adjacency sparse matrices.

There is also parallelised with Open MP libraries version of the code useful for its effective execution simultaneously in several cores within one CPU. The Open MP libraries must be installed only for the execution of this particular version of the CPD code.

1. **Project files**

The project directory contains several directories:

***\src*** — contains all the source files, \*.h libraries of the project and the main.cpp file.

***\config*** — contains all the <\*.ini > files used for the initial definition of parameters governing the execution of the corresponding CPD modules;

***\PCC\_sources*** — contains a few PCCs created based on the Voronoi tessellations of the 2D and 3D cubes. A large PCC library is published on the webpage (http://materia.team/) of the Materia software project. Please see also Readme file for the PCC Analyser Python code (<https://github.com/PRISBteam/Voronoi_PCC_Analyser>) which is part of the MATERiA codes software project;

***\PCC\_database*** — contains supplementary data files for each of the project modules containing physical parameters of various materials used for simulations;

1. **Project libraries (go above)**

The source ***\src*** directory contains several subfolders with project libraries:

***main.cpp*** file is considered a separate module, setting the simulation environment and managing the implementation of all the other project modules.

***\lib*** — directory contains all the \*.h project libraries Each of the modules is placed in the folder with the same name as its own. These subdirectories contain, in their turn, <\*.h> and <\*.cpp> files with the same name as the corresponding module, and a subdirectory named *\functions* containing libraries with all the functions used in this particular module. Besides, it contains the library SupportFunctions.h with the additional functions used in several modules, measures.h with functions for calculations of various structural measures, and another library Objects.h as the only place in the project containing all the definitions of the code-specific classes. The subdirectory \ini contains the code-specific readers of the project's \*.ini files which nedds to be amended at their any significant changes. \other — contains additional external libraries such as the simple mINI reader of the \*.ini files.

***\task*** — contains all the additional user-defined tasks written as separate functions and included in the *main.cpp*. These functions became active in the mode "TASK" instead of the "LIST" of the [simulation\_mode] option in the main.ini file.

1. **Modules (go above)**
2. **Configuration files (go above)**
3. **Tasks and Tests (go above)**
4. **Applications (go above)**

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Please feel free e-mail to Dr Elijah Borodin (Research Fellow in Materials Physics at the University of Manchester, Department of Solids and Structures) any queries relating with the code.