McCAD v1.0
User Manual

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0.1 Introduction

McCAD is a C++ library for the conversion of CAD solid models to MCNP input syntax, from Boundary Representation "BREP" to Constructive Solid Geometry "CSG". The library is written in C++ and uses CMake as a build system. It relies on Open CASCADE Technology and Boost C++ libraries. Currenlty the library is a ble to process:

- Planar solids

- cylindrical solids

- toroidal solids

The library is capable of decomposing complex solids into their constituent primitives. It produces a mapping of cell IDs on the Monte Carlo input file to the CAD volume and name of the solid as loaded from the STEP file. It also produces a mapping of void to material cells in the produced Monte Carlo input file.

General notes on usage, will become more relevant after reading sections 0.1 & 0.4:

- It is advised to run decomposition and conversion separately!. This is the main reason why the conversion is disabled by default on the McCADInput-Config.i file. Checking the decomposed CAD solids for errors or interference is always advised!

- A good practice is to decompose the model few solids at a time. This ensures a smotther decomposition, as well as makes it easier to locate the troubling solid or part of the model.

- Currently, complex hollow planar solids might result in large STEP files. It is a good practice to aid the decomposition by manually cutting the solid in two, three, or more subsolids then run McCAD on the subsolids.

- Before running the conversion, it is better to check in CAD for any interference in the model. This is especially needed if simplification of tori is enabled. A clean model will result in a conversion with less errors.

- Before running McCAD, test the conversion on parts of the model. A good practice is to convert the solids that belong to a single material together. Test converting solids with another material. Then test converting both together. This way it is much easier to trace back the source of error and correct it in CAD rather than converting the entire model and try to figure out a solution to geometry errors.

- In the volumes.i file, if the user wants a list of the CAD volumes, set *compoundIsSingleCell* to "true". While it is not desirable for the transport calculations, it gives the volume of each solid in the decomposed STEP file summed over the constituent subsolids that resulted from the decomposition.

0.2 Installation from Source

Building of the McCAD library is supported on both Linux and Windows operating systems. The library has three 3rd-party dependencies: CMake, Boost C++ libraries, and Open CASCADE Technology. CMake is the standard build system for McCAD and it comes by default with most Linux distributions as well as Windows OS. Boost C++ libraries consist of header files that are utilized for parallel processing in McCAD. Open CASCADE Technology (OCCT) is used as a geometry engine for geometrical solids manipulation and decomposition. Below are guiding steps for installation on both Linux and Win systems.

0.2.1 Linux

Listed below are the currently supported Linux distributions:

- Ubuntu 20.04 LTS

- Ubuntu 18.04 LTS

Testing of installation on other distributions is still underway! thus Ubuntu is recommended as a distribution to install McCAD. Below are general steps to install McCAD code and its dependencies.

- **CMake**
    - Download cmake-3.23.0.tar.gz from https://cmake.org/download/ then execute the commands below in a terminal.
    - $ tar -xzvf cmake-3.23.0.tar.gz
    - $ cd cmake-3.23.0
    - $ mkdir build
    - $ cd build
    - $ cmake .. -DCMAKE_USE_OPENSSL=OFF -DCMAKE_INSTALL_PREFIX=.
    - $ make
    - $ make install

- **Boost C++ liraries**
  - Download boost_1_78_0.tar.gz from https://www.boost.org/users/download/ then execute the commands below in a terminal.
  - $ tar -xvzf boost_1_78_0.tar.gz
  - $ cd boost_1_78_0
  - $ mkdir build
  - $ cd tools/build
  - $ ./bootstrap.sh
  - $ ./b2 install --prefix=../../build/

- **Open CASCADE Technology (OCCT)**
  - *NOTE*: the instructions on the installation of dependencies can be found on the side menu in https://dev.opencascade.org/doc/occt-7.5.0/overview/html/index.html by navigating to "Build, Debug and Upgrade > Build 3rd-parties" then following the instructions under "Installation from Official Repositories".
  - Download opencascade-7.5.0.tgz from https://dev.opencascade.org/release/previous then execute the commands below in a terminal.
  - $ tar -xzvf opencascade-7.5.0.tgz
  - $ cd opencascade-7.5.0
  - $ mkdir build
  - $ cd build
  - $ cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_LIBRARY_TYPE=Shared -DCMAKE_INSTALL_PREFIX=. -DINSTALL_TEST_CASES=TRUE -DINSTALL_DOC_Overview=TRUE
  - $ make
  - $ make install

- **McCAD**
  - *NOTE*: building a shared library is recommended! Should a static library be needed, the user has to insure a compliant build of Open CASCADE Technology by changing the build type; -DBUILD_LIBRARY_TYPE=STATIC.
  - $ git clone https://github.com/inr-kit/McCAD_Library
  - $ cd McCAD_Library

- $ mkdir build

- $ cd build

- $ CMake .. -DCMAKE_INSTALL_PREFIX=. -DBUILD_STATIC=OFF -DBOOST_CUSTOM_ROOT=<PATH to boost_1_78_0> -DOCC_CUSTOM_ROOT=<P to opencascade-7.5.0/build> -DBUILD_RPATH=ON

- $ make

- $ make install

0.2.2 Windows

Listed below are the currently supported Windows versions:

- Windows 10

Testing of installation on other versions is still underway! Below are general steps to build McCAD library and its dependencies.

- **CMake** (optional)

  - *NOTE*: If usage of IDE - such Microsoft Visual Studio (VS) - is intended, then installing CMake can be skipped since most IDE builds CMake by default.

  - Download and run the installer cmake-3.23.1-windows-x86_64.msi from https://cmake.org/download/.

- **Microsoft Visual Studio** (optional)

  - Download and run the "community" installer from https://visualstudio.microsoft.com/downloads/.

- **Boost C++ liraries**

  - Download boost_1_78_0.zip from https://www.boost.org/users/download/.

  - Unzip boost_1_78_0.zip.

  - Documentation can be found in index.html in the unzipped folder.

- **Open CASCADE Technology (OCCT)**

  - Download and run the installer opencascade-7.5.0-vc14-64.exe from https://dev.opencascade.org/release/previous.

- **McCAD**

- Download source code from https://github.com/inr-kit/McCAD_Library by selecting Code > Download ZIP.
- Unzip McCAD_Library.
- Open MSVC and select the McCAD_Library.
- From the "Solution Explorer - Folder Review" double click CMakeSettings.json file. This will open the file in IDE.
- Set a "Configuration name".
- Ensure that "Configuration type" is set to "Release" and "Toolset" is set to msvc_x64_x64.
- Add -DBUILD_RPATH=ON -DBUILD_STATIC_EXE=ON -DBUILD_SHARED=OFF -DBOOST_CUSTOM_ROOT="<PATH to boost_1_78_0>" -DOCC_CUSTOM_ROOT=" to OpenCASCADE-7.5.0-vc14-64\opencascade-7.5.0>" to "CMake command arguments".
- From the top menu select "Build > Build All".
- From the top menu select "Build > Install McCAD".

0.3 I/O

In general, there are three types of information that need to be provided to McCAD: geometry model(s), materials assignment, and running parameters. Below, the input pertinent to the decomposition and conversion will be highlighted. The output from McCAD will depend on the mode of execution, as will be described in the following sections.

0.3.1 General

The first input to be provided is the input configuration file, McCADInputConfig.i. When run via a command line *without arguments*, McCAD will generate a template configuration file, figure (1), with the default values of the run parameters. In both run modes, decomposition and conversion, McCAD input parameters are needed. The run parameters are assigned values by default and can be modified by the user. Below is a description of the general input parameters.

- **debugLevel**: the level at which run/debug info is diplayed on the screen. *Default* is 0.

- **units**: The units used in the CAD model. *Default* is cm.

- **inputFileName**: the input STEP file(s) name(s). *Default* is input.stp.

0.3.2   Decomposition

Currently McCAD supports input files in the STEP format (protocol 214). Mc-CAD accepts both single and multiple input STEP files. After successfully running McCAD decomposition two STEP output files will be written to disk. The first will contain the decomposed input solids and the second will contain the rejected/failed input solids. If the latter is absent, this means no input solids were rejected and no solids failed to be decomposed.

Before running McCAD in the decomposition mode, the user is advised to review the input parameters on the decomposition section on the input configuration file, figure (1). Below is a description of the decomposition input parameters.

- **decompose**: a logical condition for running decomposition on the input file(s). *Default* is true.

- **recurrenceDepth**: defines the level of decomposition performed recursively on input solids. This input specifies the maximum number of recursive application of decomposition on the subsolids. The larger the number, the less the failed solids with a lot of detailes in the geometry. *Default* is 20.

- **minSolidVolume**: this input is used to control the recursive splitting of the solids along with the reciurrenceDepth. It is also used to filter the input solids by rejecting smaller solids than the specified value. *Default* is 1.0e-3 cm^3.

- **minFaceArea**: used to filter the input solids by rejecting solids with faces smaller in area than the specified value. *Default* is 1.0e-4 cm^2.

- **scalingFactor**: controls the size of generated mesh on solids faces. This parameter mainly affects the collision detection of surfaces. More details can be found in section **??**. *Default* is 100.0.

- **precision**: used to judge the equality of numerical values. *Default* is 1.0e-6.

- **faceTolerance**: More details can be found in section **??**. *Default* is 1.0e-8 cm.

- **edgeTolerance**: More details can be found in section **??**. *Default* is 1.0e-8 cm.

- **parameterTolerance**: More details can be found in section **??**. *Default* is 1.0e-8 cm.

- **angularTolerance**: More details can be found in section **??**. *Default* is 1.0e-4 radian/PI.

- **distanceTolerance**: More details can be found in section **??**. *Default* is 1.0e-6 cm.

- **simplifyTori**: a logical condition on whether or not simplify toroidal solids as a collection of smaller cylindrical segments. If true, only off axis tori will be simplified. *Default* is false.

- **simplifyAllTori**: a logical condition on whether or not simplify all toroidal solids as a collection of smaller cylindrical segments. If true, all toroidal solids, disregarding its axis, will be simplified. *Default* is false.

- **torusSplitAngle**: the angle between the top and bottom bases of a cylindrical segment. *Default* is 30.0 degrees.

0.3.3 Conversion

McCAD conversion will result in three textual output files. The first contains the generated Monte Carlo, MCNP is only support for now, input file. The second contains a mapping of cell ID, volume, and solid name. The third file contains a mapping of void cell IDs to material cell IDs. More details on the format of the three files can be found in section **??**.

Material assignment is currently deduced from the name of the STEP files. The user is advised to split the CAD model into several by material. The name of the input STEP files takes the format <material name><density in exponential format: -0.0E0><.stp. The material name and density are then extracted from the file name and assigned to the solids it contains. For MCNP, the sign of the density implies whether mass or atomic densities is used. In case of absence of the density value, void is assumed. It is important to note that the underscore only separates the material name from density. Any extra underscores will result in an error.

Before running McCAD in the conversion mode, the user is advised to review the input parameters on the conversion section on the input configuration file, figure (1). Below is a description of the decomposition input parameters.

- **convert**: a logical condition for running conversion on the input file(s). *Default* is false.

- **voidGeneration**: a logical condition for void generation. If false, only a single void cell is created outside which is a graveyard. *Default* is false.

- **compoundIsSingleCell**: controls whether to define the subsolids of the decomposid input solid into separate cells or unify it through the union operator into a single cell. If true, all subsolids are joined through a union operator and a single cell is written to the MC input file. This is not recommended for complex solids since it slows down the transport due to the many surface crossing checks. *Default* is false.

- **minVoidVolume**: controls the desirable minimum void cell volume. *Default* is 1.0 cm^3.

- **maxSolidsPerVoidCell**: this input will control the number of generated void cells. A smaller number will result in a larger number of void cells each with simpler expression on the MC file. *Default* is 40.

- **BVHVoid**: a logical condition for generating a bound volume hierarchy void cells. This feature is still undergoing testing and not currently recommended to be used. *Default* is false.

- **MCcode**: specifies the targeted MC code to generate the input file in a compliant format. Currently only MCNP is supported. *Default* is mcnp.

- **startCellNum**: the desired starting cell number. *Default* is 1.

- **startSurfNum**: the desired starting surface number. *Default* is 1.

- **startMatNum**: the desired starting material number. *Default* is 1.

- **maxLineWidth**: maximum length of lines on the MC file. *Default* is 80.

- **MCFileName**: the desired name for the MC file. *Default* is MCFile.i.

- **volumesFileName**: the desired name for the cell ID-volumes-name mapping file. *Default* is volumes.i.

- **voidCellsFileName**: the desired name of the void to material cells mapping file. *Default* is voidCells.i.

0.4 Running McCAD

There are two ways to run McCAD, via a command line or the SpaceClaim plugin. McCAD can be run from a command line either in a Linux terminal or a Windows command prompt.

0.4.1 Command Line

On a linux termial of Windows command prompt McCAD can be run by typing in the path to the executable followed by the desired argument. A good practice is to add the path to the McCAD executable to the PATH environment variable then simply call McCAD with the acceptable desired command line arguments. The arguments could be displayed on the screen by running "McCAD help". The acceptable McCAD arguments are listed below.

- []: running McCAD without arguments will result in writing McCAD template input configuration file, McCADInputConfig.i.

- [**help**]: lists all the acceptable arguments.

- [**read**]: test loading the solids from the input STEP file(s). This is used to test if the OCCT reader will fail to load any STEP file(s).

- [**run**]: executes McCAD according to the selected running mode: decomposition, conversion, or both.

0.4.2 SpaceClaim Plugin

The python script located in plugins/SpaceClaim_interface can be loaded into SpaceClaim and used directly to call McCAD to perform decomposition on selected solid(s). The script can be loaded in SPaceClaim by selecting "File > New > Script". Select the desired solid(s) to decompose and on the "Script Editor" select "Run Script", the green arrow.

0.5 Example

This section will discuss how to run McCAD. The example input STEP file as well as the output files can be found in examples/collection_of_solids folder. The input file, SS_-793e-2.stp, contains a collection of random solids, as shown in figure (2); with steps, cylinders, tori, protrusions, depressions, etc. The solids from the file are assigned stainless steel material (SS) with a density of 7.93 g/cm^3.

1. With the path to McCAD executable added to the PATH environment variable, the McCADInputConfig.i file could be generated by running McCAD, without any arguments, figure (3).

2. On McCADInputConfig.i file, the *inputFileName* should be changed to SS_-793e-2.stp. Also, *convert* and *voidGeneration* parameters should be set to "true".

3. McCAD is then run via the command "McCAD run". After successfully running McCAD there should be a total of 4 new files generated on disk. Figure (4) shows the displayed output of McCAD on screen for decomposition and conversion.

   - The first file is produced by McCAD decomposition algorithm, SS_-793e-2Decomposed.stp, and contains the decomposed input solids. Upon loading the file into any CAD software we could see the decomposed solids, as shown in figure (5).

   - The second file is produced by McCAD conversion algorithm, MCFile.i. The file is the MCNP input file and contains cell, surface,data cards in MCNP format, figure (6).

   - The third file is produced by McCAD conversion algorithm, volumes.i. The file lists cell IDs, volumes of solids, and name on the CAD STEP file, figure (7).

   - The fourth file is produced by McCAD conversion algorithm, voidCells.i. The file maps void to material cell IDs, figure (8).

0.6 Known Issues

A list of known issues and how to manually fix it in solid models. Coming soon ...

0.6.1 Decomposition

- coordinates

- simplifying of tori

- hollow solids

- splitting of cylinders and tori

0.6.2 Conversion

0.7 Theory of McCAD Conversion

A comperhensive discussion on the inner workings of McCAD algorithm/classes for developers. Coming soon ...

0.7.1 Decomposition

0.7.2 Conversion

```
# McCAD Run Parameters    Mon May 23 17:10:46 2022
# ====================

# Input
# =====
# > Debug level: 0, 1, 2, 3. [0] provides no debugging outputs.
debugLevel = 0
# > The unit used for the input STEP file(s).
units = cm
# > Path to the input STEP file;
inputFileName = input.stp

# Decomposition
# =============
decompose = true
recurrenceDepth = 20
minSolidVolume = 1.0e-3 [cm3]
minFaceArea = 1.0e-4 [cm2]
scalingFactor = 100.0
precision = 1.0e-6
faceTolerance = 1.0e-8 [cm]
edgeTolerance = 1.0e-8 [cm]
parameterTolerance = 1.0e-8 [cm]
angularTolerance = 1.0e-4 [radian/PI]
distanceTolerance = 1.0e-6 [cm]
simplifyTori = false
simplifyAllTori = false
torusSplitAngle = 30.0 [degrees]

# Conversion
# ==========
convert = false
# > Choose whether or not to generate void cells;
voidGeneration = false
# > Condition to treat a compound as a single cell or a group of cells.
compoundIsSingleCell = false
# > Minimum acceptable void volume shouldn;t be less than minSolidVolume;
minVoidVolume = 1.0 [cm3]
# > A larger number will result in fewer void cells but longer cell expressions;
maxSolidsPerVoidCell = 40
# > Choose whether or not to generate Bound Volume Heirarchy void cells;
BVHVoid = false
# > Choose the desired MC code for conversion;
MCcode = mcnp
startCellNum = 1
startSurfNum = 1
startMatNum = 1
maxLineWidth = 80
MCFileName = MCFile.i
volumesFileName = volumes.i
voidCellsFileName = voidCells.i
```

Figure 1: McCAD Input Configuration File
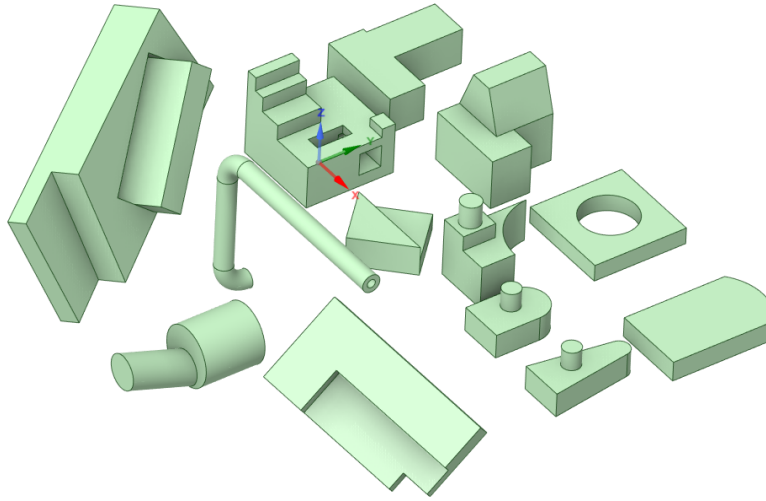
Figure 2: Example Input Solids

Figure 3: McCAD Output

(a)

(b)

Figure 4: McCAD Decomposition (a) and Conversion (b) Displayed Outputs
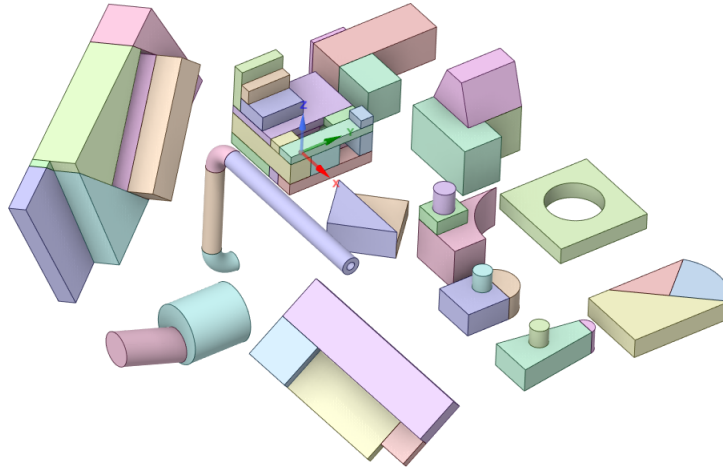
Figure 5: McCAD Decomposed Input Solids

Figure 6: McCAD Generated MCFile.i File

```
McCAD v1.0 generated volumes file. Wed May 11 15:39:53 2022
Column 1 is the cell ID, column 2 is the volume [cubic cm], and column 3 is the compound name.
1 5.83682E-01 COMPOUND
2 1.83520E+00 COMPOUND
3 2.13120E-01 COMPOUND
4 4.47330E+00 COMPOUND
5 1.78503E+00 COMPOUND
6 1.20204E+00 COMPOUND
7 1.04096E+00 COMPOUND
8 3.59000E-01 COMPOUND
9 6.55000E-01 COMPOUND
10 6.54400E-01 COMPOUND
11 1.74406E+00 COMPOUND
12 6.54400E-02 COMPOUND
13 1.20162E+00 COMPOUND
14 1.11720E+00 COMPOUND
15 1.88183E+00 COMPOUND
16 1.08619E+00 COMPOUND
17 3.54465E+00 COMPOUND
18 2.42556E+00 COMPOUND
19 8.14044E-03 COMPOUND
20 9.52734E-01 COMPOUND
21 1.52089E-01 COMPOUND
22 7.77544E-02 COMPOUND
23 1.21200E+00 COMPOUND
24 9.92320E-01 COMPOUND
25 3.20923E-01 COMPOUND
26 4.68008E-01 COMPOUND
27 5.36000E-01 COMPOUND
28 5.20248E-02 COMPOUND
29 2.10487E-01 COMPOUND
30 7.04021E-01 COMPOUND
31 5.20248E-02 COMPOUND
32 3.41412E-02 COMPOUND
33 6.41431E-01 COMPOUND
34 1.73887E+00 COMPOUND
35 2.40000E-02 COMPOUND
36 2.45000E-01 COMPOUND
37 8.22500E-02 COMPOUND
38 2.56500E-01 COMPOUND
39 4.86200E-01 COMPOUND
40 2.80500E-02 COMPOUND
```

Figure 7: McCAD Generated volumes.i File

```
McCAD v1.0 generated void - material cell IDs mapping file. Wed May 11 15:39:53 2022
Column 1 is the void cell ID and column(s) 2(+) is(are) the material cell ID(s).
55    5 6 7 8 9 10 11 12 14 15 16 17 18 19 20 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54
56    1 2 3 4 8 9 13 21 22 23 24 25 26 27 28 29 30 31 32 33 34 52
```

Figure 8: McCAD Generated voidCells.i File