CompuCell3D Developers Manual Documentation

Release 1.0.0

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FUNDING

The focus of this manual is to explain internals of C++ code and provide all information you need start writing your own C++ extension modules for CompuCell3D

CHAPTER

ONE

FUNDING

From early days CompuCell3D was funded by science grants. The list of funding entities include

- National Institutes of Health (NIH)
- US Environmental Protection Agency (EPA)
- National Science Foundation (NSF)
- Falk Foundation
- Indiana University (IU)
- IBM

The development of CC3D was funded fully or partially by the following awards:

- National Institutes of Health, National Institute of Biomedical Imaging and Bioengineering,U24 EB028887, "Dissemination of libRoadRunner and CompuCell3D", (09/30/2019 – 06/30/2024)
- National Science Foundation, NSF 1720625, "Network for Computational Nanotechnology - Engineered nanoBIO Node", (09/1/2017-08/31/2022)
- National Institutes of Health, National Institute of General Medical Sciences, R01 GM122424, "Competitive Renewal of Development and Improvement of the Tissue Simulation Toolkit", (02/01/2017 - 01/31/2021)
- Falk Medical Research Trust Catalyst Program, Falk 44-38-12, "Integrated in vitro/in silico drug screening for ADPKD", (11/30/2014-11/29/2017)
- National Institutes of Health, National Institute of General Medical Sciences, National Institute of Environmental Health Sciences and National Institute of Biomedical Imaging and Bioengineering, U01 GM111243 "Development of a Multiscale Mechanistic Simulation of Acetaminophen-Induced Liver Toxicity", (9/25/14-6/30/19)
- National Institutes of Health, National Institute of General Medical Sciences, R01 GM076692, "Competitive Renewal of MSM: Multiscale Studies of Segmentation in Vertebrates", (9/1/05-8/31/18)
- U. S. Environmental Protection Agency, R835001, "Ontologies for Data & Models for Liver Toxicology", (6/1/11-5/30/15)
- National Institutes of Health, National Institute of General Medical Sciences, R01 GM077138, "Competitive Renewal of Development and Improvement of the Tissue Simulation Toolkit", (9/1/07-3/31/15).
- U. S. Environmental Protection Agency, National Center for Environmental Research, R834289, "The Texas-Indiana Virtual STAR Center: Data-Generating in vitro and in silico Models of Development in Embryonic Stem Cells and Zebrafish", (11/1/09-10/31/13)
- Pervasive Technologies Laboratories Fellowship (Indiana University Bloomington) (12/1/03-11/30/04).
- IBM Innovation Institute Award (9/25/03-9/24/06)

- National Science Foundation, Division of Integrative Biology, IBN-0083653, “BIOCOMPLEXITY–Multiscale Simulation of Avian Limb Development”, (9/1/00-8/31/07)

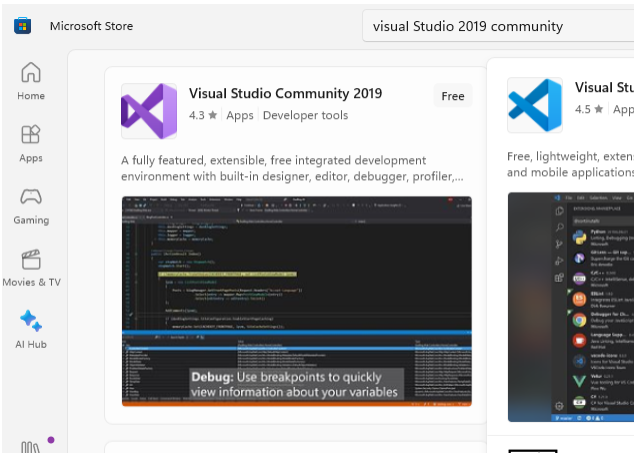
CHAPTER

TWO

WINDOWS

In order to compile entire CC3D code on Windows (not just the developer zone) you need to install Visual Studio 2015 Community Edition (free). Here is a reference page on how to find the relevant installation bundles. Make sure you use CommunityEdition: https://stackoverflow.com/questions/44290672/how-to-download-visual-studio-community-edition-2015-not-2017

You can also install Visual Studio 2019 from Microsoft Store. Both of those frameworks should work fine when it comes to compilation of CC3D code. One thing to remember that is you want to recompile the code it is often a good idea to close and reopen Visual Studio because otherwise compilations may take a long time and your IDE may even freeze - no matter how fast your computer is



Once you installed Visual Studio 2015 Community Edition or Visual Studio 2019 Community Edition (you may need to restart your computer after the installation is finished) you need to install Miniconda3 from heere: https://docs.conda.io/projects/miniconda/en/latest/

Once you install the latest version of Miniconda for your operating system you should install mamba into `base` conda environment:

```
conda install -c conda-forge mamba
```

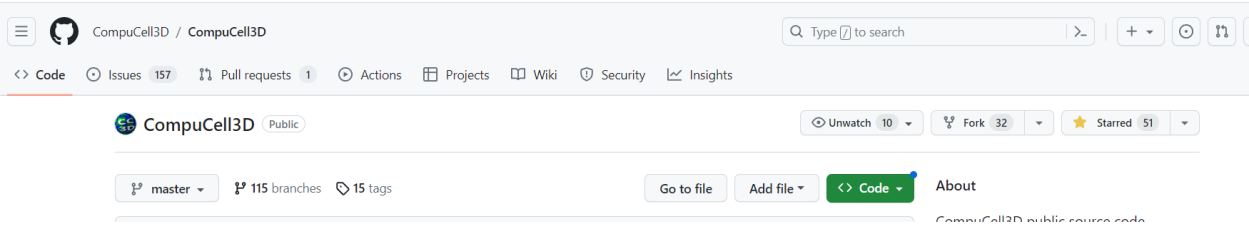
Note, `-c conda-forge` points to `conda-forge` channel that is one of the most reliable repositories of conda packages.

Note

If you are just interested in building CompuCell3D and do not plan to contribute to CompuCell3D code, you can simply clone CompuCell3D repository, bypassing the forking step described below. Simply run the following commands

```
cd d:/src/
git clone https://github.com/CompuCell3D/CompuCell3D.git
```

Next fork CompuCell3D core code repository from https://github.com/CompuCell3D/CompuCell3D. Simply log in to your github account, navigate to the CompuCell3D link and click Fork button in the upper right corner of the page:



Once you forked the code, go ahead and clone it from your repository (not from CompuCell3D repository).

To clone repository you follow command pattern below:

```
cd d:/src/
git clone git@github.com:<your_github_name>/CompuCell3D.git
```

Now we are ready to start configuring CompuCell3D build. The entire process of setting up code build for CC3D is based on conda-recipe that we use to build conda packages. It might be worth looking at the content of `D:/src/CompuCell3D/conda-recipes/` directory , in particular at the `D:/src/CompuCell3D/conda-recipes/bld.bat` file. We will leverage content of this file to construct invocation of the `cmake` command that will set up compilation of CompuCell3D in Visual Studio 2015.

Note

I assumed that my forked repository was cloned to `D:/src/CompuCell3D`. If you cloned it to a different folder you will need to adjust paths accordingly

At this point we need to prepare conda environment that has all dependencies needed to compile CC3D. The main ones include Python and the VTK library, but there are many others so instead of listing them all here, let's leverage conda packages that we use to distribute CompuCell3D. Those key packages that are required to compile CC3D are stored in the conda environment file below. Copy the content of this file ave it as env310.yaml. I saved mine to `D:src\env310.yaml`

```
name: cc3d_4413_310
channels:
  - conda-forge
  - compucell3d
dependencies:
  - python=3.10
  - numpy=1.24
  - vtk=9.2
  - eigen
  - tbb-devel=2021
  - boost=1.78
  - cmake>=3.28
  - swig=4
  - psutil
```

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```
  - deprecated
  - cc3d-network-solvers>=0.3.0
  - scipy
  - pandas
  - jinja2
  - simservice
  - notebook
  - ipywidgets
  - ipyvtklink
  - sphinx
  - graphviz
  - qscintilla2
  - webcolors
  - requests
  - pyqt=5
  - pyqtgraph
  - pyqtwebkit
  - chardet
  - fipy
```

Notice the first line `name: cc3d_4413_310` specifies the name oft the conda environment this file will create - it will be called `cc3d_4413_310`

Next two lines specify conda channels (repositories) from which the packages listed in the file will be downloaded from

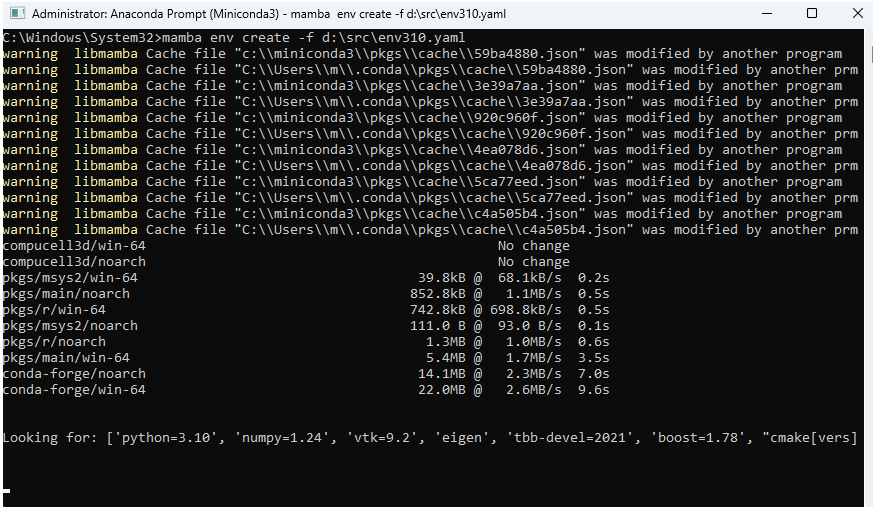
```
channels:
  - conda-forge
  - compucell3d
```

Here we list conda packages repositories. conda-forge is by far the most popular and package-rich conda package repository and compucell3d is the repository that stores dependencies needed to install or build compucell3d. The `dependencies` section lists all packages needed to build core C++ Compucell3D code. NOtice we specify particular python version 3.10. It is important to know which version of python you are building packages for otjherwise you may see unexpected runtime surprises so always pay attention to nuances like this.

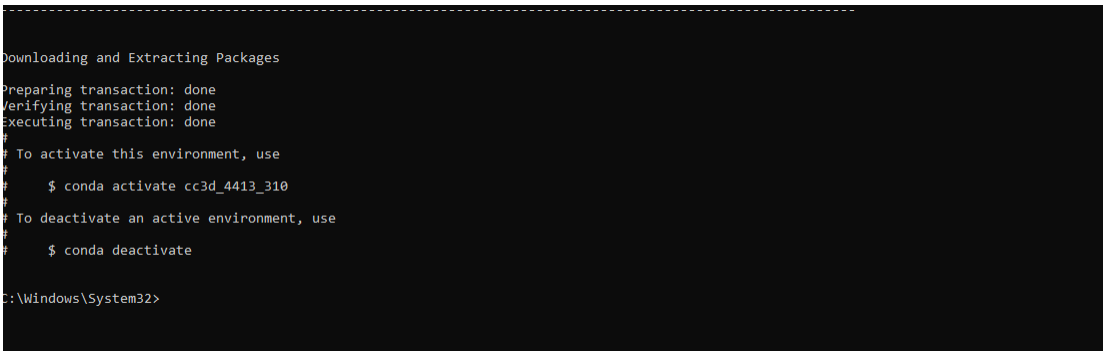
Let's use this file to actually create conda environment. Open miniconda console and run the following command:

```
mamba env create -f d:\src\env310.yaml
```

the terminal output will look similar to the one below:



and after everything is installed we will get the prompt to activate newly created conda environment conda



Note

if you are having troubles running mamba - for example if you get permission error you may need to perform conda creation in the Administrator mode or adjust permissions for your entire miniconda installation

Let's activate newly created conda environment (from now on you should be able to use regular console , not the one that runs in the Administrator mode)

```
conda activate cc3d_4413_310
```

We are ready to call `cmake` to configure CC3D C++ code compilation. Open up a new file in your editor and paste the following cmake invocation. If you are using Visual Studio 2015 the code snippet looks as follows:

```
cmake -S d:\src\CompuCell3D\CompuCell3D -B d:\src\CompuCell3D_build -DPython3_
↪EXECUTABLE=c:\miniconda3\envs\cc3d_4413_310\python.exe -DNO_OPENCL=ON  -DBUILD_
↪STANDALONE=OFF -G "Visual Studio 14 2015 Win64" -DCMAKE_INSTALL_PREFIX=D:\install_
↪projects\cc3d_4413_310
```

For Visual Studio 2019 you would use

```
cmake -S d:\src\CompuCell3D\CompuCell3D -B d:\src\CompuCell3D_build -DPython3_
↪EXECUTABLE=c:\miniconda3\envs\cc3d_4413_310\python.exe -DNO_OPENCL=ON  -DBUILD_
```

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```
↪STANDALONE=OFF -G "Visual Studio 16 2019" -DCMAKE_INSTALL_PREFIX=D:\install_projects\
↪cc3d_4413_310
```

the difference is for the `-G` option. Let's see below what each option means

GPU Solvers

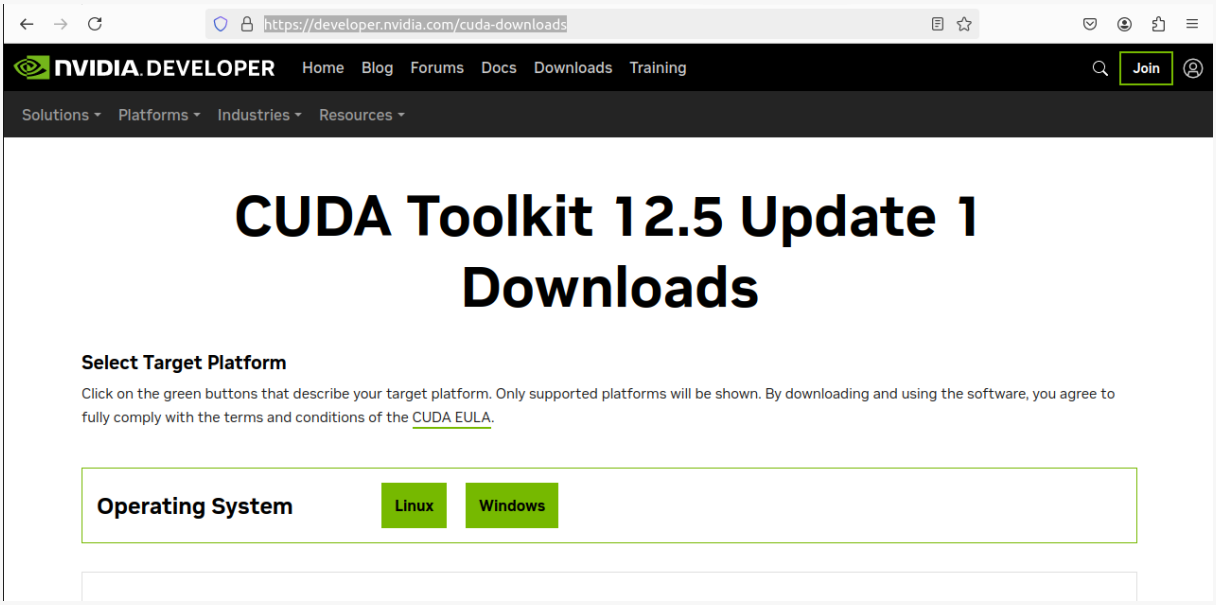
If you would like to enable GPU solvers we recommend that you use Visual Studio 2019 and the cmake command would look as follows

```
cmake -S d:\src\CompuCell3D\CompuCell3D -B d:\src\CompuCell3D_build -DPython3_
↪EXECUTABLE=c:\miniconda3\envs\cc3d_4413_310\python.exe -DNO_OPENCL=OFF  -DBUILD_
↪STANDALONE=OFF -G "Visual Studio 16 2019" -DCMAKE_INSTALL_PREFIX=D:\install_projects\
↪cc3d_4413_310
```

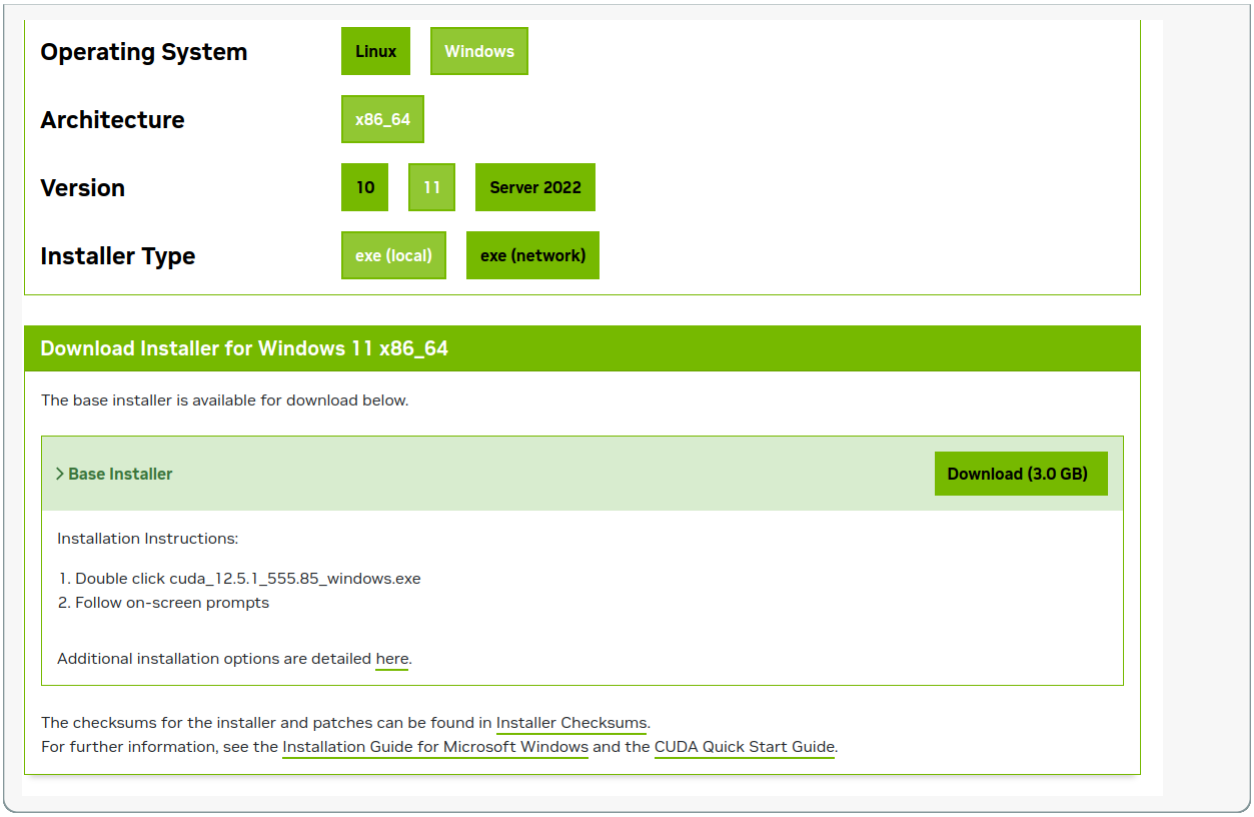
The only difference here is the `-DNO_OPENCL=OFF` option that tells Cmake system to include OpenCL modules.

Note

In order for GPU solvers to work you need to have a computer with a GPU and install GPU Toolkit. For example if you have a computer with NVidia RTX 30x0 or 40x0 card you would install Nvidia CUDA toolkit and this would be sufficient to get your GPU solvers compiled and running on your machine. Simply navigate to https://developer.nvidia.com/cuda-downloads:



select Windows and fill the details for Architecture, Version and Installer Type of your Windows - in our case we selected windows, x86_64, 11, exe (local) and follow the instruction given on the download page



Let us explain what each setting/flag means.

`-S` option allows you to specify the directory that stores and entry CMakeLists.txt file. In my case it is located in `d:\src\CompuCell3D\CompuCell3D` where `d:\src\CompuCell3D` is a path to repository and inside this folder there is `CompuCell3D` subfolder that stores CMakeLists.txt file.

`-B` option specifies where the build files are written to. The build files include intermediate compiler outputs but also Visual Studio project that we will open in the Visual Studio IDE.

-G specifies Cmake generator. CMake can generate project files for multiple IDEs and build system. Here we are specifying `Visual Studio 14 2015 Win64` so that CMake can generate VS 2015 project for Win64. For Visual Studio 2019 you use `Visual Studio 16 2019` . To get the list of all available Cmake generators type the following:

```
cmake --help
```

The next set of options all begin with `-D`. `-D` is used to set variables that are defined in CMakeLists.txt files or that are standard CMake variables. Let's go over those:

`-DPython3_EXECUTABLE=c:\miniconda3\envs\cc3d_4413_310\python.exe` - here we specify path to python executable. The `Python3_EXECUTABLE` is defined inside CMake package that sets up all Python related paths and we need to only specify python executable

`-DNO_OPENCL=ON` - specifies that we do not want to build GPU diffusion solvers. This is the variable that we introduced
`-DBUILD_STANDALONE=OFF` - this is a flag that determines how the output files will be arranged. If we use `OFF` setting plugin steppable and python bindings will be installed into miniconda environment directly. If we switch it to `ON` those plugins will be installed into `D:\install_projects\cc3d_4413_310`. If you are OK with modifying your conda environment - set it to `OFF` if not set it to `ON`. Still not all libraries will be moved to conda environment upon install and you will have to copy libraries (`.dll`) from `d:\install_projects\cc3d_4413_310\bin\` to `c:\miniconda3\envs\cc3d_4413_310\Library\bin\`

> **Note**
>
> You will need to do file copy operation after each compilation followed by Install step. It is a bit of the inconvenience but we will fix it in the future release

`-DCMAKE_INSTALL_PREFIX=D:\install_projects\cc3d_4413_310` sets standard CMake variable tha specifies installation directory.

Obviously you may need to adjust paths so that they correspond to your file system layout. If you need a template for the above command here it is:

```
cmake -S <PATH TO CompuCell3D REPO>\CompuCell3D -B <dir to store build files> -DPython3_
↪EXECUTABLE=<python executable - from conda environment> -DNO_OPENCL=ON  -DBUILD_
↪STANDALONE=OFF -G "Visual Studio 14 2015 Win64" -DCMAKE_INSTALL_PREFIX=<dir where␣
↪compiled CompuCell3D will be written to>
```

After we execute the above command (with paths adjusted to your file system layout) we will get the output that looks something as follows:

```
(cc3d_4413_310) D:\src> cmake -S d:\src\CompuCell3D\CompuCell3D -B d:\src\CompuCell3D_
↪build -DPython3_EXECUTABLE=c:\miniconda3\envs\cc3d_4413_310\python.exe -DNO_OPENCL=ON ␣
↪-DBUILD_STANDALONE=OFF -G "Visual Studio 14 2015 Win64" -DCMAKE_INSTALL_PREFIX=D:\
↪install_projects\cc3d_4413_310
-- Selecting Windows SDK version 10.0.14393.0 to target Windows 10.0.22621.
-- The C compiler identification is MSVC 19.0.24215.1
-- The CXX compiler identification is MSVC 19.0.24215.1
-- Detecting C compiler ABI info
-- Detecting C compiler ABI info - done
-- Check for working C compiler: C:\Program Files (x86)\Microsoft Visual Studio 14.0\VC\
↪bin\x86_amd64\cl.exe - skipped
-- Detecting C compile features
-- Detecting C compile features - done
-- Detecting CXX compiler ABI info
-- Detecting CXX compiler ABI info - done
-- Check for working CXX compiler: C:\Program Files (x86)\Microsoft Visual Studio 14.0\
↪VC\bin\x86_amd64\cl.exe - skipped
-- Detecting CXX compile features
-- Detecting CXX compile features - done
-- Found OpenMP_C: -openmp (found version "2.0")
-- Found OpenMP_CXX: -openmp (found version "2.0")
-- Found OpenMP: TRUE (found version "2.0")
openmp c flags -openmp
openmp cxx flags -openmp
-- Found Python3: c:\miniconda3\envs\cc3d_4413_310\python.exe (found version "3.10.12")␣
↪found components: Interpreter Development NumPy Development.Module Development.Embed
Python3_FOUND: TRUE
Python3_Interpreter_FOUND: TRUE
Python3_VERSION: 3.10.12
Python3_Development_FOUND: TRUE
Python3_EXECUTABLE: c:\miniconda3\envs\cc3d_4413_310\python.exe
Python3_Development_FOUND: TRUE
Python3_INCLUDE_DIRS: C:\miniconda3\envs\cc3d_4413_310\include
Python3_LIBRARIES: C:\miniconda3\envs\cc3d_4413_310\libs\python310.lib
```

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```
Python3_LIBRARY_RELEASE: C:\miniconda3\envs\cc3d_4413_310\libs\python310.lib
Python3_LIBRARY_DIRS: C:\miniconda3\envs\cc3d_4413_310\libs
Python3_RUNTIME_LIBRARY_DIRS: C:\miniconda3\envs\cc3d_4413_310
Python3_NumPy_INCLUDE_DIRS: C:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\numpy\
↪core\include
 THIS IS COMPUCELL3D_BUILD_VERSION 1
COMPUCELL3D_C_BUILD_VERSION is 1
GOT VERSION AS 4.4.1
-- Found ZLIB: C:\miniconda3\envs\cc3d_4413_310\Library\lib\z.lib (found version "1.2.13
↪")
 PUBLIC UTILS OPEN MP FLAG-openmp
expat library local C:\miniconda3\envs\cc3d_4413_310\Library\lib\expat.lib
-- D:\src\CompuCell3D\CompuCell3D
CMake Warning (dev) at core\CompuCell3D\steppables\PDESolvers\FindEigen3.cmake:73:
  Syntax Warning in cmake code at column 35

  Argument not separated from preceding token by whitespace.
Call Stack (most recent call first):
  core\CompuCell3D\steppables\PDESolvers\CMakeLists.txt:15 (find_package)
This warning is for project developers.  Use -Wno-dev to suppress it.

'LOCATEDEIGENAT',C:\miniconda3\envs\cc3d_4413_310\Library\include\Eigen3
-- Found Eigen3: C:\miniconda3\envs\cc3d_4413_310\Library\include\Eigen3 (Required is at␣
↪least version "2.91.0")
-- OpenCL disabled
OPENMP FLAGS -openmp
-- Found SWIG: C:\miniconda3\envs\cc3d_4413_310\Library\bin\swig.exe (found version "4.1.
↪1")
-- Found Python3: c:\miniconda3\envs\cc3d_4413_310\python.exe (found suitable version "3.
↪10.12", minimum required is "3.10") found components: Interpreter Development.Module␣
↪Development.Embed
-- Looking for pthread.h
-- Looking for pthread.h - not found
-- Found Threads: TRUE
-- Found GLEW: C:\miniconda3\envs\cc3d_4413_310\Library\lib\glew32.lib
-- Found OpenGL: opengl32  found components: OpenGL
-- Found HDF5: hdf5-shared (found version "1.14.2") found components: C HL
-- Found utf8cpp: C:\miniconda3\envs\cc3d_4413_310\Library\include
-- Found JsonCpp: C:\miniconda3\envs\cc3d_4413_310\Library\lib\jsoncpp.lib (found␣
↪suitable version "1.9.5", minimum required is "0.7.0")
-- Found OGG: C:\miniconda3\envs\cc3d_4413_310\Library\lib\ogg.lib
-- Found THEORA: C:\miniconda3\envs\cc3d_4413_310\Library\lib\theora.lib
-- Found NetCDF: C:\miniconda3\envs\cc3d_4413_310\Library\include (found version "4.9.2")
-- Found LibPROJ: C:\miniconda3\envs\cc3d_4413_310\Library\lib\proj.lib (found version
↪"9.2.1")
-- Found LibXml2: C:\miniconda3\envs\cc3d_4413_310\Library\lib\xml2.lib (found version
↪"2.11.5")
-- Found GL2PS: C:\miniconda3\envs\cc3d_4413_310\Library\lib\gl2ps.lib (found suitable␣
↪version "1.4.2", minimum required is "1.4.2")
-- Found PNG: C:\miniconda3\envs\cc3d_4413_310\Library\lib\libpng.lib (found version "1.
↪6.39")
-- Found nlohmann_json: C:\miniconda3\envs\cc3d_4413_310\Library\share\cmake\nlohmann_
```

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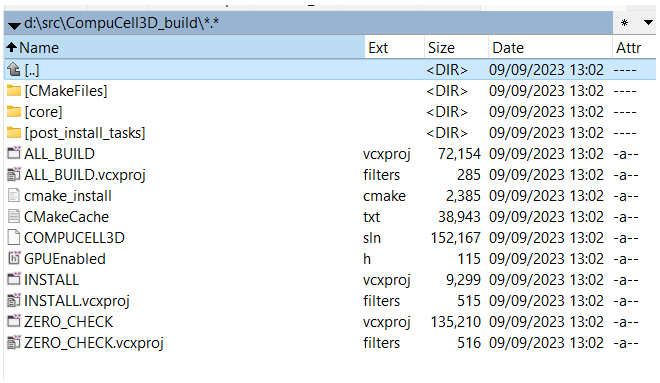
```
↪json\nlohmann_jsonConfig.cmake (found version "3.11.2")
-- Found SQLite3: C:\miniconda3\envs\cc3d_4413_310\Library\include (found version "3.43.0
↪")
-- Found Eigen3: C:\miniconda3\envs\cc3d_4413_310\Library\include\eigen3 (found version
↪"3.4.0")
-- Found EXPAT: C:\miniconda3\envs\cc3d_4413_310\Library\lib\expat.lib (found version "2.
↪5.0")
-- Found double-conversion: C:\miniconda3\envs\cc3d_4413_310\Library\lib\double-
↪conversion.lib
-- Found LZ4: C:\miniconda3\envs\cc3d_4413_310\Library\lib\liblz4.lib (found version "1.
↪9.4")
-- Found LZMA: C:\miniconda3\envs\cc3d_4413_310\Library\lib\liblzma.lib (found version
↪"5.4.2")
-- Found JPEG: C:\miniconda3\envs\cc3d_4413_310\Library\lib\jpeg.lib (found version "80")
-- Found TIFF: C:\miniconda3\envs\cc3d_4413_310\Library\lib\tiff.lib (found version "4.5.
↪1")
-- Found Freetype: C:\miniconda3\envs\cc3d_4413_310\Library\lib\freetype.lib (found␣
↪version "2.12.1")
VTK_MAJOR_VERSION=9
NUMPY_INCLUDE_DIR
VTK_LIB_DIRS
THIS IS cc3d_py_source_dir: D:\src\CompuCell3D\CompuCell3D\..\cc3d
USING EXTERNAL PYTHON
-- Configuring done
CMake Warning (dev) at compucell3d_cmake_macros.cmake:200 (ADD_LIBRARY):
  Policy CMP0115 is not set: Source file extensions must be explicit.  Run
  "cmake --help-policy CMP0115" for policy details.  Use the cmake_policy
  command to set the policy and suppress this warning.

  File:

    D:\src\CompuCell3D\CompuCell3D\core\CompuCell3D\steppables\PDESolvers\hppppdesolvers.h
Call Stack (most recent call first):
  core\CompuCell3D\steppables\PDESolvers\CMakeLists.txt:187 (ADD_COMPUCELL3D_STEPPABLE)
This warning is for project developers.  Use -Wno-dev to suppress it.

-- Generating done
-- Build files have been written to: D:\src\CompuCell3D_build
```

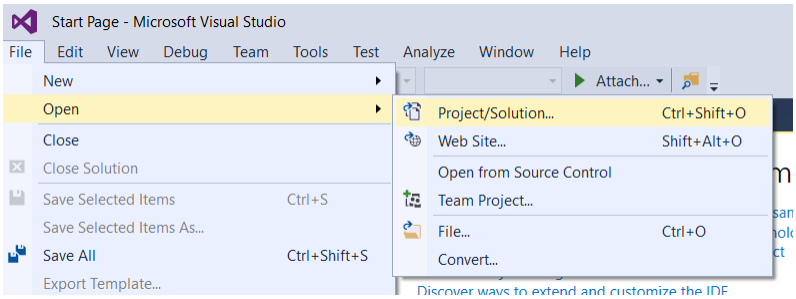
Note

If your output does not look like this, ensure that you are using the same environment for the entire tutorial, including every instance in your CMake command and every place that you copy compiled files to

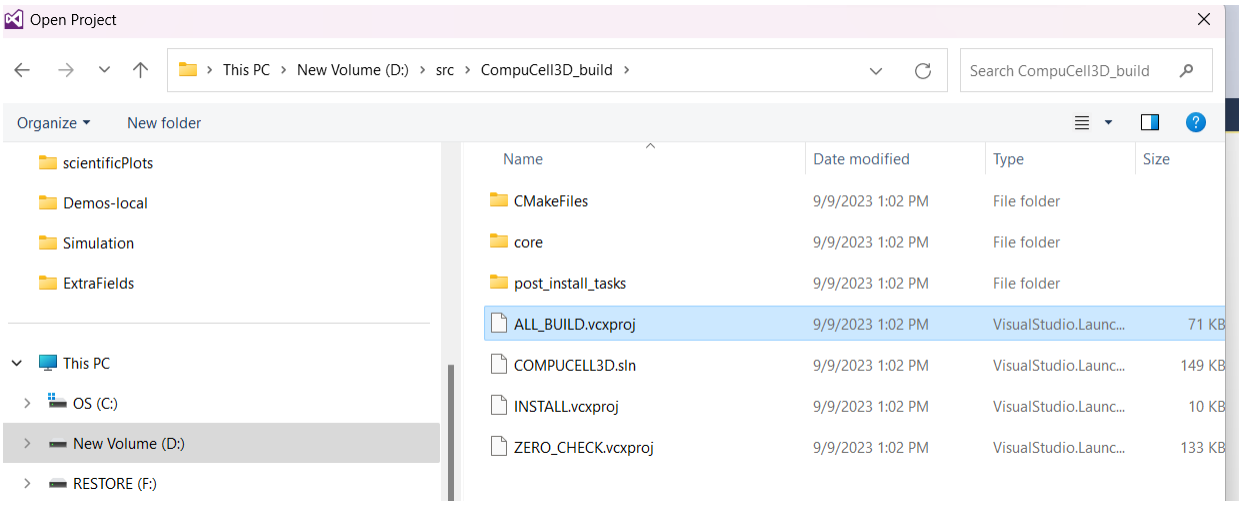
The line `-- Generating done` shows `-- Build files have been written to: D:\src\CompuCell3D_build`.



At this point we can open the newly generated project in the Visual Studio 2015 IDE and start compilation. In Visual Studio 2015 navigate to `File->Open...->Project/Solution...`

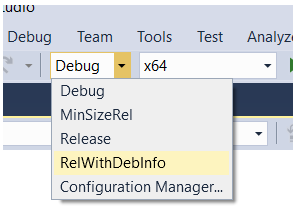


and navigate to where VS 2015 files are generated and pick `ALL_BUILD.vcxproj`

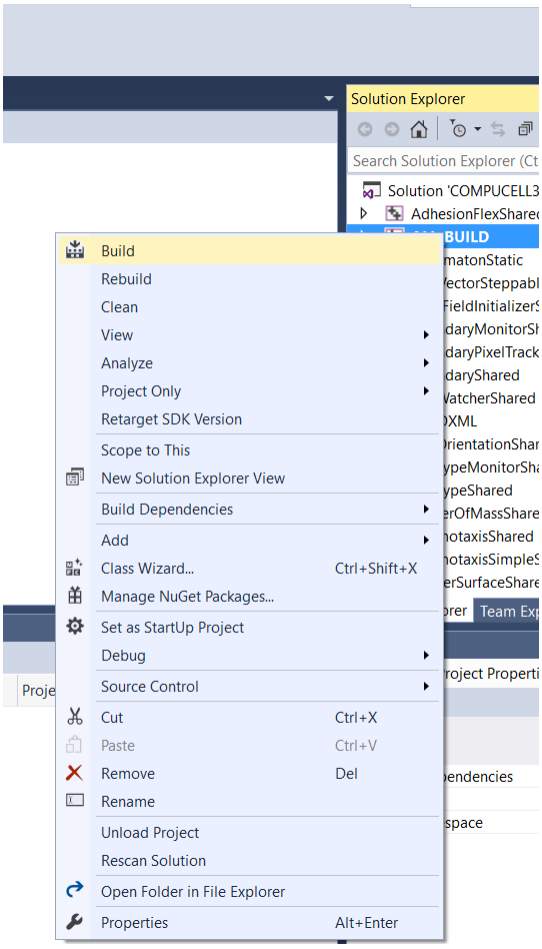


Once the project is loaded we set compile configration (we choose RelWithDebInfo from the pull-down menu)

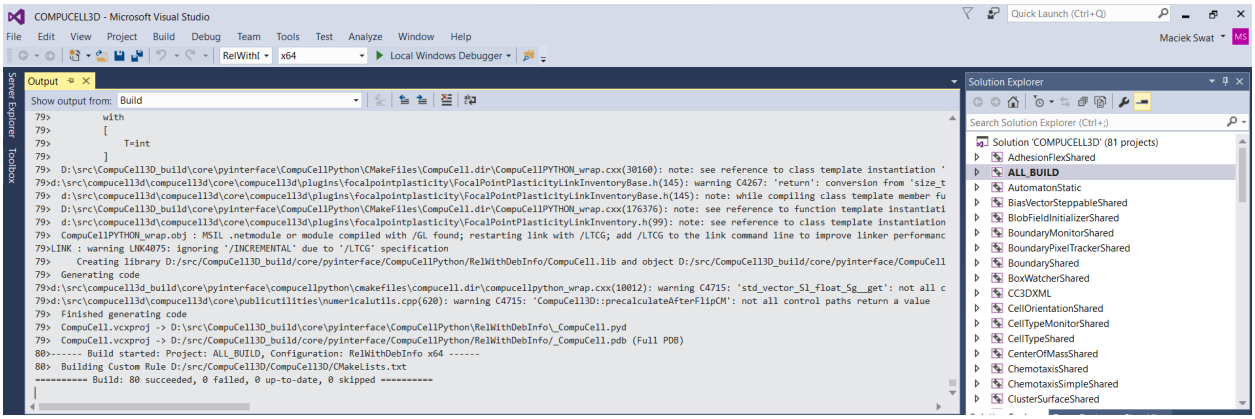
> **Note**
>
> If you have compilation errors, you may try again with Release mode instead of RelWithDebInfo.



Next, from the `Solution Explorer` panel, right-click on `ALL_BUILD` and select `Build` from context menu

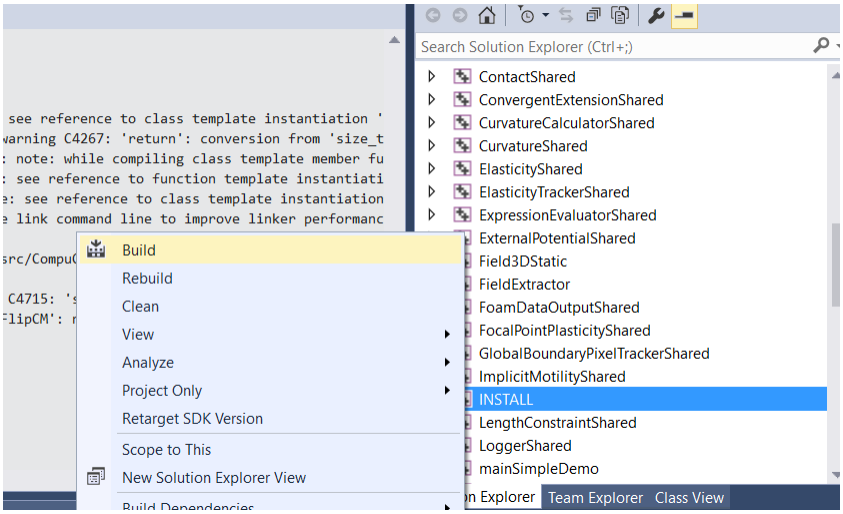


The compilation will start and after a while (say 10-15 minutes on Windows , much faster on other platforms) you will get compilation completion screen

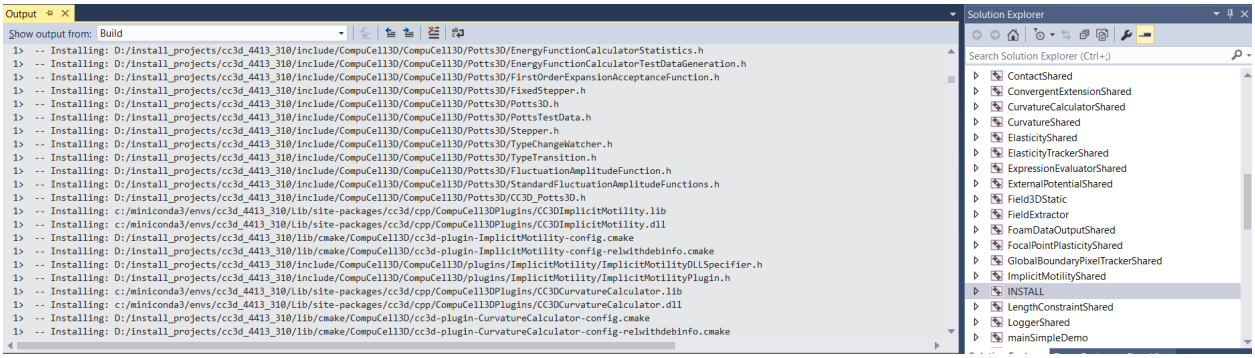


Once compilation succeeded, go ahead and install all the libraries to the target dir:

Find `INSTALL` subproject in the `Solution Explorer`, right-click and choose `Build` to install all the libraries:



and if you take a look at the output screen you will see that some files are installed into `d:\install_projects\cc3d_4413_310` and some are written directly into conda environment `c:\miniconda3\envs\cc3d_4413_310`

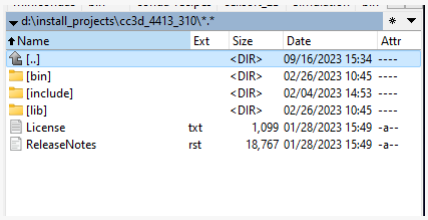


At this point your newly compiled CC3D shold be ready to use

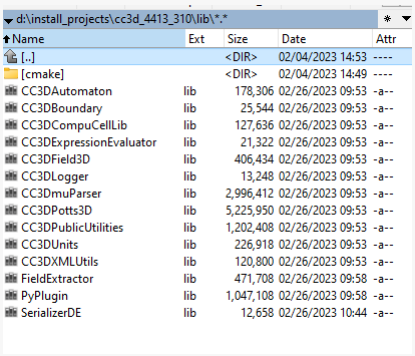
Note

The following steps apply to releases before `4.6.0` , as of `4.6.0` you do not need to follow those steps.

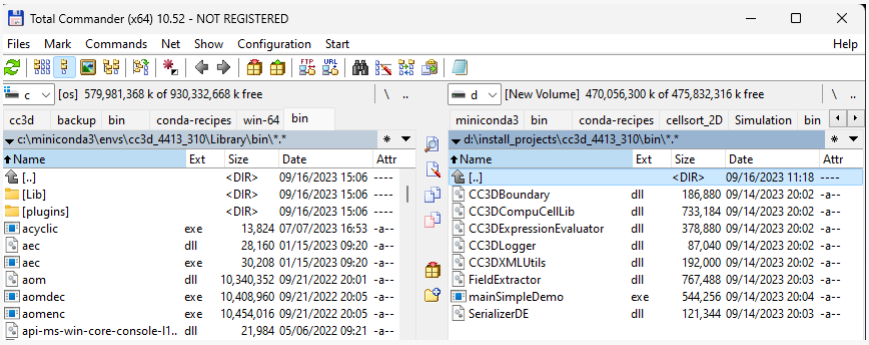
After installation step the `d:\install_projects\cc3d_4413_310\` directory will look something like



and if we look into `d:\install_projects\cc3d_4413_310\lib` we see no `site-packages` because `site-packages` that contains ``cc3d` package has been installed directly into conda environment - hence no need to perform manual copy



The only thing that remains now is to copy dlls from `d:\install_projects\cc3d_4413_310\bin\` to `c:\miniconda3\envs\cc3d_4413_310\Library\bin\` See the section "Changing layout of installed CC3C C++ code" for more details.



At this point your conda environment will contain binaries that are coming from your compiled version of CompuCell3D.

2.1 Manually installing Player and Twedit ++

Once you installed CC3D to miniconda environment `cc3d_4413_310` all that you need to get Player and Twedit working with yor new environment is to clone those repos

```
cd d:\src
git clone https://github.com/CompuCell3D/cc3d-player5.git
git clone https://github.com/CompuCell3D/cc3d-twedit5.git
```

and copy `d:\src\cc3d-player5\cc3d\player5` folder to `c:\miniconda3\envs\cc3d_4413_310_develop\Lib\site-packages\cc3d\player5\` and similarly, compy `d:\src\cc3d-twedit5\cc3d\twedit5` folder to `c:\`

`miniconda3\envs\cc3d_4413_310_develop\Lib\site-packages\cc3d\twedit5\`

2.2 Running Newly Compiled CC3D

At this point you can open Player or Twedit through Miniconda prompt (make sure you are still in the cc3d_4413_310 environment)

```
python -m cc3d.player5
```

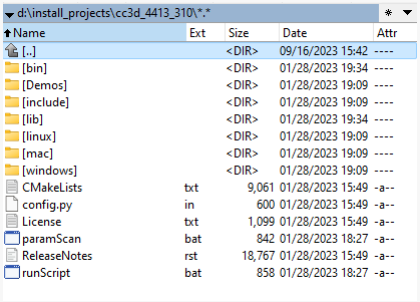
2.3 Using newly compiled binaries with the UI

Follow this guide to setup PyCharm to run the Player and use your newly compiled C++ code - *Running Player and Twedit++ from PyCharm*.

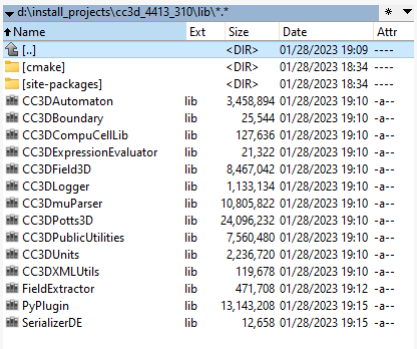
Note

This is legacy material that no longer applies to current version of CC3D but is relevant when users want to compile earlier CC3D versions

To Change the layout of the C++ code we could use `-DBUILD_STANDALONE=ON` option and if we do that and repeat all the steps we showed in this writeup you will end up with the layout of the install directory that looks as follows:



and if we look into `d:\install_projects\cc3d_4413_310\lib` we actually we see `site-packages`



so in this case we need copy `d:\install_projects\cc3d_4413_310\lib\site-packages` into `c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\`

For this example, I am working on new steppable plugin called MyModule. Each time you make changes to the code, do the following:

1. Right-click the module you edited in Visual Studio's Solution Explorer, click Project Only -> Build Only MyModule. If you modified core files, such as Potts, then you should use ALL_BUILD instead of Project

Only.

2. Right click INSTALL, then click Build in Solution Explorer.
3. Edit the below batch script for your machine's directories. Additionally, if you had set `-DBUILD_STANDALONE=ON`, then you may skip Step 2.

```
echo "Step 1: Copy all .dll files from bin"
cd d:\install_projects\bin\
cp *.dll c:\miniconda3\envs\cc3d_4413_310\Library\bin\

echo "Step 2: Copy site-packages"
mkdir c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d
cp -r d:\install_projects\lib\site-packages\cc3d\* c:\miniconda3\envs\
↪cc3d_4413_310\Lib\site-packages\cc3d

echo "Step 3: Copy .lib files"
cd d:\install_projects\lib\
cp *.lib c:\miniconda3\envs\cc3d_4413_310\Library\lib\

echo "Done"
pause
```

CHAPTER

THREE

MAC - OSX

In order to compile entire CC3D code on Mac (not just the developer zone) you need to install OSX core developer tools:

```
xcode-select --install
```

For CompuCell3D development we also need miniconda installation - please follow instructions from Miniconda website: https://docs.anaconda.com/free/miniconda/

Next let's install `mamba` which give you much faster package dependency resolution. Open new terminal and tun the following:

```
conda install -c conda-forge mamba
```

Note

We will use ~ to denote home directory. This is standard Linux/Unix/OSX convention On my computer miniconda is installed to `~/miniconda_arm64` folder. It is likely that on yours it will be a different folder so please make a note of this because later we will need the location of the miniconda to configure compilation of CompuCell3D

Once you have those tools you are ready to create conda environment into which we will install all the libraries and compilers that are needed for CC3D compilation. There are multiple ways to handle the installation of those prerequisites but the easiest one is to use `environment.yaml` files where we list all needed packages and provide this file to conda which takes care of installing them.

Note

From now on I will assume that all git repositories and files have been saved to `~/src-cc3d`, that is to `src-cc3d` folder placed inside your home directory (~)

First, let's clone CompuCell3D, cc3d-player5 and cc3d-twedit5 git repositories to `!/src-cc3d`

```
mkdir -p ~/src-cc3d
cd ~/src-cc3d
git clone https://github.com/CompuCell3D/CompuCell3D.git
git clone https://github.com/CompuCell3D/cc3d-player5.git
git clone https://github.com/CompuCell3D/cc3d-twedit5.git
```

Next, let's create file `~/src-cc3d/environment.yaml` with the following content:

```yaml
channels:
  - conda-forge
  - compucell3d
dependencies:
# compile dependencies
    - cmake=3.21
    - swig>=4
    - numpy=2.2.6
    - clang_osx-arm64
    - clangxx_osx-arm64
    - llvm-openmp
    - python=3.12
    - vtk=9.2
    - eigen
    - tbb-devel=2021
    - boost=1.85
    - psutil
    - deprecated
    - cc3d-network-solvers>=0.3.1
# cc3d run dependencies
    - simservice
    - notebook
    - ipywidgets
    - ipyvtklink
    - sphinx
    - graphviz
    - scipy
    - pandas
    - jinja2
# player dependencies
    - webcolors
    - requests
    - pyqt=5
    - pyqtgraph
# twedit dependencies
    - chardet
    - pyqtwebkit
    - qscintilla2
    - sphinx
    - pywin32 # [win]
```

Note

To generate this environment.yaml file it is best to to start the conda build process of cc3d package and navigate to the `work` folder within conda-bld directory and then copy all packages from the `metadata_conda_debug.yaml` file e.g. in my case the file I used was `~/miniconda3_arm64/conda-bld/cc3d_1711231453909/work/metadata_conda_debug.yaml`. The important thing is to copy this file away from this folder while the conda build still runs (otherwise after successful build this file will disappear) and to remove duplicates from the package list. We also added few packages that Player and Twedit++ use. They are not necessary to compile CompuCell3D but they will be useful later when we will run CompuCell3D via `cc3d-player`

Once we created `environment.yaml` let's `cd` to `~/src-cc3d` and create environment called `cc3d_compile` by run-

ning the following command:

```
cd ~/src-cc3d
mamba env create -f environment.yaml --name cc3d_compile
```

The output of of the last command should look something like this

```
  + yarl                                          1.9.4  py310hd125d64_0        conda-
↪forge/osx-arm64     Cached
  + zeromq                                        4.3.5  hebf3989_1             conda-
↪forge/osx-arm64     Cached
  + zipp                                         3.17.0  pyhd8ed1ab_0           conda-
↪forge/noarch        Cached
  + zlib                                         1.2.13  h53f4e23_5             conda-
↪forge/osx-arm64     Cached
  + zstd                                          1.5.5  h4f39d0f_0             conda-
↪forge/osx-arm64     Cached

  Summary:

  Install: 337 packages

  Total download: 0 B



Downloading and Extracting Packages

Preparing transaction: done
Verifying transaction: done
Executing transaction: \
/
done
#
# To activate this environment, use
#
#     $ conda activate cc3d_compile
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

After environment in installed let's activate this environment - as suggested but above printout by running:

```
conda activate cc3d_compile
```

At this point we are ready to configure CompuCell3D for compilation. We will be using CMake.

Let's run the following command:

```
cmake -S ~/src-cc3d/CompuCell3D/CompuCell3D -B ~/src-cc3d/CompuCell3D_build -DPython3_
↪EXECUTABLE=$CONDA_PREFIX/bin/python -DNO_OPENCL=ON  -DBUILD_STANDALONE=OFF -G "Unix␣
↪Makefiles" -DCMAKE_INSTALL_PREFIX=~/src-cc3d/CompuCell3D_install
```

Let's explain command line arguments we used when calling `cmake` command

`-S` - specifies location of the CompUCdl3D source code and the actual C++ code resides indeed in `~/src-cc3d/CompuCell3D/CompuCell3D`

`-B` specifies the location of the temporary compilation files

`-DPython3_EXECUTABLE=` specifies the location of the python interpreter. Notice that it points to the conda environment we creates (`/envs/cc3d_compile/bin/python`). **Important:** We used `$CONDA_PREFIX` env var to point to the conda environment we have just activated. In my case it points to `/Users/m/miniconda3_arm64/envs/cc3d_compile`. In your case it will be different but ouu can always check by executing `echo $CONDA_PREFIX` from the terminal where you activate `cc3d_compile` environment

``-DNO_OPENCL=ON `` - is a CC3D-specific setting that tells cmake to skip generating GPU diffusion solvers. Note, the support for OpenCL on OSX is/might be problematic, hence we are using morte conservative setting and skip generation of those solvers

`-DBUILD_STANDALONE=OFF` - is a CC3D-specific setting that tells cmake to install all python packages to python interpreter directory - i.e. inside `$CONDA_PREFIX` (e.g. `/Users/m/miniconda3_arm64/envs/cc3d_compile`)

`-DCMAKE_INSTALL_PREFIX=` specifies location of installed CompuCell3D binaries

`-G "Unix Makefiles"` instructs cmake to generate unix Makefiles that we will use for compilation of CompuCell3D

After running the las t command the output should look as follows:

```
...
-- Found Freetype: /Users/m/miniconda3_arm64/envs/cc3d_compile/lib/libfreetype.dylib␣
↪(found version "2.12.1")
VTK_MAJOR_VERSION=9
NUMPY_INCLUDE_DIR
VTK_LIB_DIRS
THIS IS cc3d_py_source_dir: /Users/m/src-cc3d/CompuCell3D/CompuCell3D/../cc3d
USING BUNDLE
-- Configuring done
CMake Warning (dev) at compucell3d_cmake_macros.cmake:200 (ADD_LIBRARY):
  Policy CMP0115 is not set: Source file extensions must be explicit.  Run
  "cmake --help-policy CMP0115" for policy details.  Use the cmake_policy
  command to set the policy and suppress this warning.

  File:

    /Users/m/src-cc3d/CompuCell3D/CompuCell3D/core/CompuCell3D/steppables/PDESolvers/
↪hpppdesolvers.h
Call Stack (most recent call first):
  core/CompuCell3D/steppables/PDESolvers/CMakeLists.txt:187 (ADD_COMPUCELL3D_STEPPABLE)
This warning is for project developers.  Use -Wno-dev to suppress it.

-- Generating done
-- Build files have been written to: /Users/m/src-cc3d/CompuCell3D_build
(cc3d_compile) m@Maciejs-MacBook-Pro src-cc3d %
```

At this point we are ready to compile CC3D:

```
cd ~/src-cc3d/CompuCell3D_build
make -j 8
```

We are changing to the "build directory" where or cmake, Makefile, and transient compilation files are stored and we are running `make` command with 8 parallel compilation threads to speed up the compilation process. The successful compilation printout should look something like that:

```
[ 99%] Linking CXX shared module _PlayerPython.so
[ 99%] Built target PlayerPythonNew
16 warnings generated.
[100%] Linking CXX shared module _CompuCell.so
[100%] Built target CompuCell
```

After the compilation is done we will call ``*make install*

```
make install
```

The installed files will be placed in `~/src-cc3d/CompuCell3D_install` , exactly as we specified in the `cmake` command - `-DCMAKE_INSTALL_PREFIX=~/src-cc3d/CompuCell3D_install`

Assuming we are still in cc3d_compile conda environment (run `conda activate cc3d_compile` if you opened new terminal) we can run our first simulation using newly compiled CompuCell3D. We will run it without the player first and next we will show you how to get player and twedit++ working.

```
python -m cc3d.run_script -i ~/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/
↪cellsort/cellsort_2D/cellsort_2D.cc3d
```

Note

First time you execute run command on OSX it takes a while to load all the libraries. Subsequent runs start much faster

The output of the run should look something like this

```
(cc3d_compile) m@Maciejs-MacBook-Pro CompuCell3D_build % python -m cc3d.run_script -i ~/
↪src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/cellsort/cellsort_2D/cellsort_2D.
↪cc3d
#################################################
# CompuCell3D Version: 4.5.0 Revision: 2
 Commit Label: f8ddda9
#################################################
<cc3d.core.CC3DSimulationDataHandler.CC3DSimulationData object at 0x12de43a00>
Random number generator: MersenneTwister
WILL RUN SIMULATION FROM BEGINNING
CALLING FINISH


------------------PERFORMANCE REPORT:----------------------
-----------------------------------------------------------
TOTAL RUNTIME 9 s : 639 ms = 9.639 s
-----------------------------------------------------------
-----------------------------------------------------------
PYTHON STEPPABLE RUNTIMES
            cellsort_2DSteppable:        0.01 ( 0.1%)
-----------------------------------------------------------
            Total Steppable Time:        0.01 ( 0.1%)
    Compiled Code (C++) Run Time:        9.54 (99.0%)
                      Other Time:        0.08 ( 0.9%)
-----------------------------------------------------------
```

3.1 Using Player

To run the above simulation using player we need to make player code available to the Python interpreter from which we are running our simulation. In my case this will boil down to either copying directory `~/src-cc3d/cc3d-player5/cc3d/player5` inside `$CONDA_PREFIX/lib/python3.1/site-packages/cc3d/player5`

or making a softlink. I prefer the softlink and I run:

```
ln -s ~/src-cc3d/cc3d-player5/cc3d/player5   $CONDA_PREFIX/lib/python3.1/site-packages/
↪cc3d/player5
```

After this step I am ready to run previous simulation using the Player:

```
python -m cc3d.player5
```

and then we would use `File->Open...` menu to select our `.cc3d` project `~/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/cellsort/cellsort_2D/cellsort_2D.cc3d`

CHAPTER

FOUR

LINUX - UBUNTU

In order to compile entire CC3D code on Linux (not just the developer zone) you need to miniconda. Once you have this tool it will take care of installing all the dependencies you need to to compie CC3D

Follow instructions from Miniconda website: https://docs.anaconda.com/free/miniconda/

Next let's install `mamba` which give you much faster package dependency resolution. Open new terminal and tun the following:

```
conda install -c conda-forge mamba
```

Once you have those tools you are ready to create conda environment into which we will install all the libraries and compilers that are needed for CC3D compilation. There are multiple ways to handle the installation of those prerequisites but the easiest one is to use `environment.yaml` files where we list all needed packages and provide this file to conda which takes care of installing them.

Note

From now on I will assume that all git repositories and files have been saved to `/home/m/src-cc3d` . You may want to adjust this path so that it corresponds to working folder that exists on your file system. In all commands below you would replace `/home/m/src-cc3d` with the folder of your choice.

First, let's clone CompuCell3D, cc3d-player5 and cc3d-twedit5 git repositories to `/home/m/src-cc3d`

```
mkdir -p /home/m/src-cc3d
cd /home/m/src-cc3d
git clone https://github.com/CompuCell3D/CompuCell3D.git
git clone https://github.com/CompuCell3D/cc3d-player5.git
git clone https://github.com/CompuCell3D/cc3d-twedit5.git
```

Next, let's create file `/home/m/src-cc3d/environment.yaml` with the following content:

```
channels:
  - conda-forge
  - compucell3d
dependencies:
 # compile dependencies
  - cmake=3.21
  - swig>=4
  - numpy=1.24
  - gcc_linux-64
  - gxx_linux-64
```

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```
  - python 3.10
  - vtk=9.2
  - eigen
  - tbb-devel=2021
  - boost=1.85
# libxcrypt dependency was discovered during actual compilation - searched pkgs sub-
↪folders for all occurrences of crypt.h
  - libxcrypt
  - psutil
  - deprecated
  - cc3d-network-solvers>=0.3.0
# cc3d run dependencies
  - scipy
  - pandas
  - jinja2
  - deprecated
  - psutil
  - simservice
  - notebook
  - ipywidgets
  - ipyvtklink
  - sphinx
  - graphviz
# player dependencies
  - webcolors
  - requests
  - pyqt=5
  - pyqtgraph
# twedit dependencies
  - chardet
  - pyqtwebkit
  - qscintilla2
  - pywin32 # [win]
```

Once we created `environment.yaml` let's `cd` to `/home/m/src-cc3d` and create environment called `cc3d_compile` by running the following command:

```
cd /home/m/src-cc3d
mamba env create -f environment.yaml --name cc3d_compile
```

The output of of the last command should look something like this

```
  ...
  + xorg-xproto                                7.0.31  h7f98852_1007          conda-
↪forge/linux-64     Cached
  + xz                                          5.2.6  h166bdaf_0             conda-
↪forge/linux-64     Cached
  + yaml                                        0.2.5  h7f98852_2             conda-
↪forge/linux-64     Cached
  + yarl                                        1.9.4  py310h2372a71_0        conda-
↪forge/linux-64     Cached
  + zeromq                                      4.3.5  h59595ed_1             conda-
```

(continues on next page)

(continued from previous page)

```
↪forge/linux-64     Cached
  + zipp                                            3.17.0  pyhd8ed1ab_0           conda-
↪forge/noarch       Cached
  + zlib                                            1.2.13  hd590300_5             conda-
↪forge/linux-64     Cached
  + zstd                                             1.5.5  hfc55251_0             conda-
↪forge/linux-64     Cached

  Summary:

  Install: 375 packages

  Total download: 49MB

──────────────────────────────────────────────────────────────────────────────────────────────────────



libxslt                                              254.3kB @   1.5MB/s  0.2s
ipywidgets                                           113.6kB @ 671.0kB/s  0.2s
widgetsnbextension                                   886.4kB @   2.3MB/s  0.4s
jupyterlab_widgets                                   187.1kB @ 479.9kB/s  0.4s
pywin32                                                8.2kB @  14.4kB/s  0.4s
pyqtgraph                                            695.0kB @ 983.5kB/s  0.3s
qtwebkit                                              15.6MB @   3.9MB/s  3.8s
python                                                31.3MB @   4.4MB/s  7.0s

Downloading and Extracting Packages

Preparing transaction: done
Verifying transaction: done
Executing transaction: /
-
done
#
# To activate this environment, use
#
#     $ conda activate cc3d_compile
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

After environment in installed let's activate this environment - as suggested but above printout by running:

```
conda activate cc3d_compile
```

At this point we are ready to configure CompuCell3D for compilation. We will be using CMake.

> **Note**
>
> It is important to replace `/home/m/src-cc3d` with the directory into which you cloned the three CompuCell3D repositories repository

Let's run the following command:

```
cmake -S /home/m/src-cc3d/CompuCell3D/CompuCell3D -B /home/m/src-cc3d/CompuCell3D_build -
↪DPython3_EXECUTABLE=/home/m/miniconda3/envs/cc3d_compile/bin/python -DNO_OPENCL=ON  -
↪DBUILD_STANDALONE=OFF -DOPENGL_gl_LIBRARY=/usr/lib/x86_64-linux-gnu/libGL.so -DOPENGL_
↪glx_LIBRARY=/usr/lib/x86_64-linux-gnu/libGLX.so -G "Unix Makefiles" -DCMAKE_INSTALL_
↪PREFIX=/home/m/src-cc3d/CompuCell3D_install
```

Let's explain command line arguments we used when calling `cmake` command

`-S` - specifies location of the CompUCdl3D source code and the actual C++ code resides indeed in `/home/m/src-cc3d/CompuCell3D/CompuCell3D`

`-B` specifies the location of the temporary compilation files

`-DPython3_EXECUTABLE=` specifies the location of the python interpreter. Notice that it points to the conda environment we creates (`/envs/cc3d_compile/bin/python`). **Important:** depending where you installed your miniconda you may need to replace `/home/m/miniconda3` with the path you miniconda installation on your machine

``-DNO_OPENCL=ON `` - is a CC3D-specific setting that tells cmake to skip generating GPU diffusion solvers. Note, the support for OpenCL on OSX is/might be problematic, hence we are using morte conservative setting and skip generation of those solvers

`-DBUILD_STANDALONE=OFF` - is a CC3D-specific setting that tells cmake to install all python packages to python interpreter directory - i.e. inside `/home/m/miniconda3/envs/cc3d_compile`

`-DCMAKE_INSTALL_PREFIX=` - specifies location of installed CompuCell3D binaries

`-DOPENGL_gl_LIBRARY=/usr/lib/x86_64-linux-gnu/libGL.so` - specifies location of OpenGL libraries

`-DOPENGL_glx_LIBRARY=/usr/lib/x86_64-linux-gnu/libGLX.so` - - specifies location of OpenGL libraries

`-G "Unix Makefiles"` instructs cmake to generate unix Makefiles that we will use for compilation of CompuCell3D

> **Note**
>
> The two OpenGL options (`-DOPENGL_gl_LIBRARY=/usr/lib/x86_64-linux-gnu/libGL.so` and `-DOPENGL_glx_LIBRARY=/usr/lib/x86_64-linux-gnu/libGLX.so`) work only on Ubuntu. If you are compiling CC3D on different distribution e.g RedHat you may need to adjust those. Also if you have a better solution for finding those libraries using Cmake commands please share it with us!

After running the las t command the output should look as follows:

```
...
-- Found X11: /home/m/miniconda3/envs/cc3d_compile/include
-- Looking for XOpenDisplay in /home/m/miniconda3/envs/cc3d_compile/lib/libX11.so;/home/
↪m/miniconda3/envs/cc3d_compile/lib/libXext.so
-- Looking for XOpenDisplay in /home/m/miniconda3/envs/cc3d_compile/lib/libX11.so;/home/
↪m/miniconda3/envs/cc3d_compile/lib/libXext.so - found
-- Looking for gethostbyname
-- Looking for gethostbyname - found
-- Looking for connect
-- Looking for connect - found
-- Looking for remove
-- Looking for remove - found
-- Looking for shmat
-- Looking for shmat - found
```

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```
-- Looking for IceConnectionNumber in ICE
-- Looking for IceConnectionNumber in ICE - found
-- Found EXPAT: /home/m/miniconda3/envs/cc3d_compile/lib/libexpat.so (found version "2.5.
↪0")
-- Found double-conversion: /home/m/miniconda3/envs/cc3d_compile/lib/libdouble-
↪conversion.so
-- Found LZ4: /home/m/miniconda3/envs/cc3d_compile/lib/liblz4.so (found version "1.9.4")
-- Found LZMA: /home/m/miniconda3/envs/cc3d_compile/lib/liblzma.so (found version "5.2.6
↪")
-- Found JPEG: /home/m/miniconda3/envs/cc3d_compile/lib/libjpeg.so (found version "80")
-- Found TIFF: /home/m/miniconda3/envs/cc3d_compile/lib/libtiff.so (found version "4.6.0
↪")
-- Found Freetype: /home/m/miniconda3/envs/cc3d_compile/lib/libfreetype.so (found␣
↪version "2.12.1")
VTK_MAJOR_VERSION=9
NUMPY_INCLUDE_DIR
VTK_LIB_DIRS
THIS IS cc3d_py_source_dir: /home/m/src-cc3d/CompuCell3D/CompuCell3D/../cc3d
USING BUNDLE
-- Configuring done
CMake Warning (dev) at compucell3d_cmake_macros.cmake:200 (ADD_LIBRARY):
  Policy CMP0115 is not set: Source file extensions must be explicit.  Run
  "cmake --help-policy CMP0115" for policy details.  Use the cmake_policy
  command to set the policy and suppress this warning.

  File:

    /home/m/src-cc3d/CompuCell3D/CompuCell3D/core/CompuCell3D/steppables/PDESolvers/
↪hpppdesolvers.h
Call Stack (most recent call first):
  core/CompuCell3D/steppables/PDESolvers/CMakeLists.txt:187 (ADD_COMPUCELL3D_STEPPABLE)
This warning is for project developers.  Use -Wno-dev to suppress it.

-- Generating done
-- Build files have been written to: /home/m/src-cc3d/CompuCell3D_build
```

At this point we are ready to compile CC3D:

```
cd /home/m/src-cc3d/CompuCell3D_build
make -j 8
```

We are changing to the "build directory" where or cmake, Makefile, and transient compilation files are stored and we are running `make` command with 8 parallel compilation threads to speed up the compilation process. The successful compilation printout should look something like that:

```
[ 99%] Linking CXX shared module _PlayerPython.so
[ 99%] Built target PlayerPythonNew
16 warnings generated.
[100%] Linking CXX shared module _CompuCell.so
[100%] Built target CompuCell
```

After the compilation is done we will call ``*make install*

```
make install
```

The installed files will be placed in `/home/m/src-cc3d/CompuCell3D_install` , exactly as we specified in the `cmake` command - `-DCMAKE_INSTALL_PREFIX=/home/m/src-cc3d/CompuCell3D_install`

At this point we we need to copy all `.so` files from `/home/m/src-cc3d/CompuCell3D_install/lib` to `/home/m/miniconda3/envs/cc3d_compile/lib`

```
cp /home/m/src-cc3d/CompuCell3D_install/lib/*.so /home/m/miniconda3/envs/cc3d_compile/lib
```

Assuming we are still in cc3d_compile conda environment (run `conda activate cc3d_compile` if you opened new terminal) we can run our first simulation using newly compiled CompuCell3D. We will run it without the player first and next we will show you how to get player and twedit++ working.

```
python -m cc3d.run_script -i /home/m/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/
↪cellsort/cellsort_2D/cellsort_2D.cc3d
```

Note

First time you execute run command on OSX it takes a while to load all the libraries. Subsequent runs start much faster

The output of the run should look something like this (remember to adjust all paths that start with `/home/m/src-cc3d` to you file system folders):

```
(cc3d_compile) m@tuf:~/src-cc3d/CompuCell3D_build$ python -m cc3d.run_script -i /home/m/
↪src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/cellsort/cellsort_2D/cellsort_2D.
↪cc3d
################################################
# CompuCell3D Version: 4.5.0 Revision: 2
 Commit Label: f8ddda9
################################################
<cc3d.core.CC3DSimulationDataHandler.CC3DSimulationData object at 0x7f0cfd2316f0>
Random number generator: MersenneTwister
WILL RUN SIMULATION FROM BEGINNING
CALLING FINISH


------------------PERFORMANCE REPORT:----------------------
-----------------------------------------------------------
TOTAL RUNTIME 5 s : 688 ms = 5.688 s
-----------------------------------------------------------
-----------------------------------------------------------
PYTHON STEPPABLE RUNTIMES
            cellsort_2DSteppable:        0.01 ( 0.2%)
-----------------------------------------------------------
            Total Steppable Time:        0.01 ( 0.2%)
    Compiled Code (C++) Run Time:        5.60 (98.5%)
                      Other Time:        0.08 ( 1.4%)
-----------------------------------------------------------
```

4.1 Using Player

To run the above simulation using player we need to make player code available to the Python interpreter from which we are running our simulation. In my case this will boil down to either copying directory `/home/m/src-cc3d/cc3d-player5/cc3d/player5` inside `/home/m/miniconda3_arm64/envs/cc3d_compile/lib/python3.10/site-packages/cc3d/player5`

or making a softlink. I prefer the softlink and I run:

```
ln -s /home/m/src-cc3d/cc3d-player5/cc3d/player5   /home/m/miniconda3/envs/cc3d_compile/
↪lib/python3.10/site-packages/cc3d/player5
```

After this step I am ready to run previous simulation using the Player:

```
python -m cc3d.player5
```

and then we would use `File->Open...` menu to select our `.cc3d` project `/home/m/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/cellsort/cellsort_2D/cellsort_2D.cc3d`

4.2 Enabling GPU Solvers

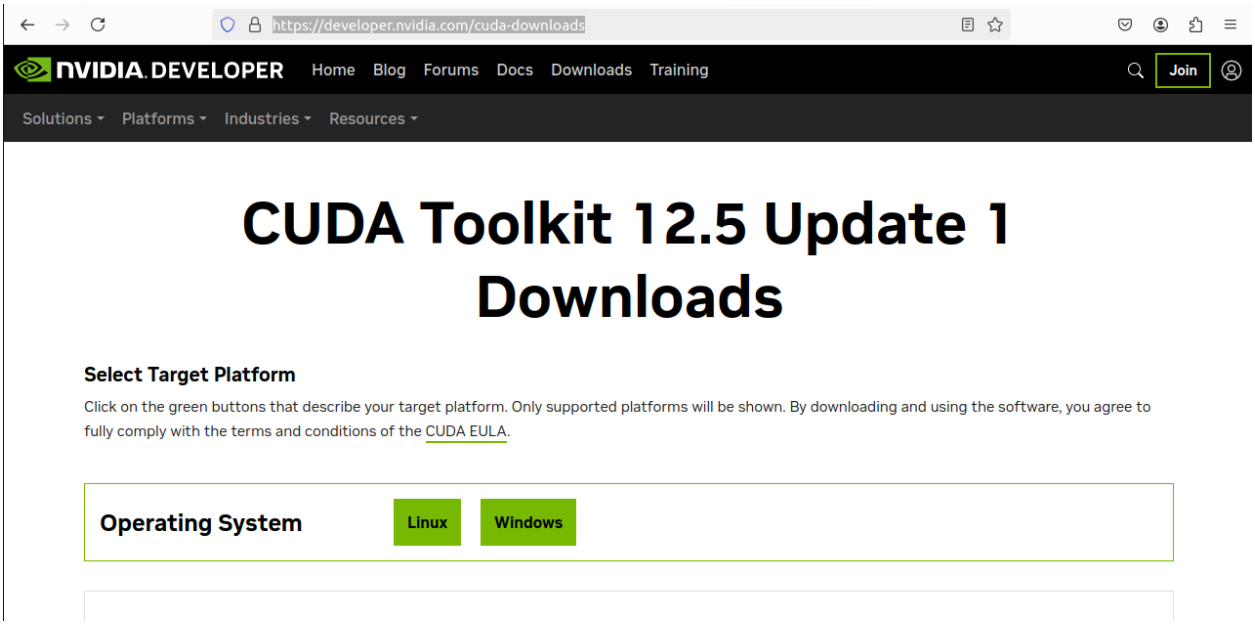
To enable GPU Solvers on your linux installation of CC3D you need to first make sure you have the right hardware on your machine. So far, we have tested CC3D with NVidia cards and the instructions we present here assume that you also have one of the NVidia GPUs. We have used Ubuntu Linux 22.04 to perform all installations but if you are using different version of Linux the compilation steps should be very simular if not identical

4.2.1 Prerequisite

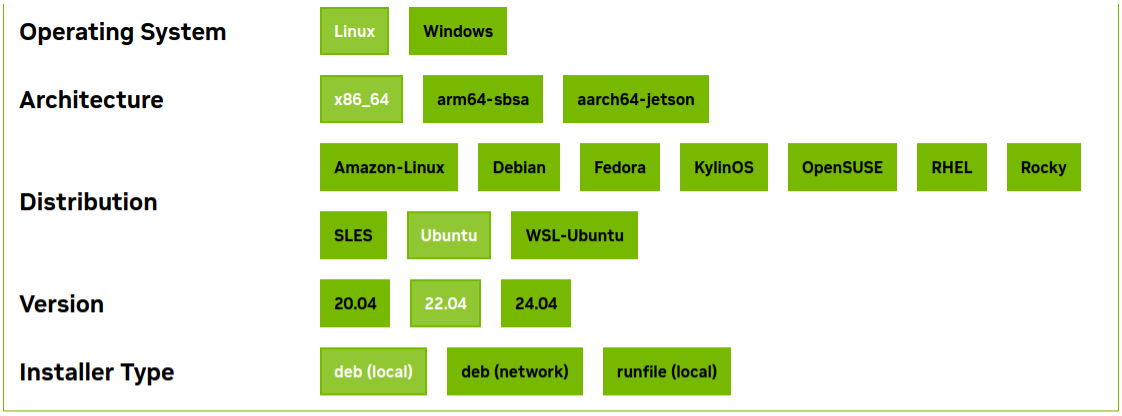
Ensure you have correct OpenCL drivers installed. Because we have NVidia hardware we used https://developer.nvidia.com/cuda-downloads to initiate the downloads for all required NVidia software that also includes OpenCL drivers.

> **Note**
>
> While Ubuntu has packages that provide CUDA and openCL support we prefer to use the latest versions of NVidia software and therefore we are downloading packages from NVidia site

After you navigate to https://developer.nvidia.com/cuda-downloads choose linux



Next, select architecture, Distribution , Version and Installer Type as appropriate - in our case we selected Linux, x86_64, Ubuntu, 22.04, deb (local) and follow the instruction as shown below:



At this point you should have all NVidia CUDA and OpenCL drivers installed. To make sure CUDA Toolkit is operational you may run

```
nvidia-smi
```

and you should see the output displaying status of your GPU device:

```
-----------------------------------------------------------------------------------------
↪+
| NVIDIA-SMI 555.42.02              Driver Version: 555.42.02      CUDA Version: 12.5   ␣
↪ |
|-----------------------------------------+------------------------+----------------------
↪-+
| GPU  Name                 Persistence-M | Bus-Id          Disp.A | Volatile Uncorr.␣
↪ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |           Memory-Usage | GPU-Util  Compute M.
↪ |
|                                         |                        |               MIG M.
↪ |
|=========================================+========================+======================|
|   0  NVIDIA GeForce RTX 3070 ...    Off |   00000000:01:00.0  On |                  N/
↪A |
| N/A   51C    P8             19W /   80W |     632MiB /   8192MiB |      4%      ␣
↪Default |
|                                         |                        |                  N/
↪A |
+-----------------------------------------+------------------------+----------------------
↪-+

+-----------------------------------------------------------------------------------------
↪-+
| Processes:                                                                             ␣
↪ |
|  GPU   GI   CI        PID   Type   Process name                             GPU␣
↪Memory |
|        ID   ID                                                              Usage      ␣
↪ |
|=========================================================================================|
```

At this point we are ready to compile CompuCell3D with the GPU solvers. This process is very similar to the "regular" CC3D compilation but we need to do one tiny hack to make sure that the correct OpenCL library gets discovered by CMake build system during the build process

Let's first create conda environment we will use for compilation - see beginning of this section for the content of the `environment.yaml`

```
cd /home/m/src-cc3d
mamba env create -f environment.yaml --name cc3d_gpu_compile
```

After the environment gets created we have to manually rename all files in `~/miniconda3/envs/cc3d_gpu_compile/lib` that start with `libOpenCL` to start with `libopenCL-x`

```
cd ~/miniconda3/envs/cc3d_gpu_compile/lib
mv libOpenCL.so libOpenCL-x.so
mv libOpenCL.so.1 libOpenCL-x.so.1
mv libOpenCL.so.1.0.0 libOpenCL-x.so.1.0.0
```

This will ensure that CMake will discover OpenCL libraries that we installed using NVidia CUDA tToolkit rather than those bundled with the miniconda

Then let's activate newly prepared conda environment:

```
conda activate cc3d_gpu_compile
```

And let's run `cmake` to initiate build process

```
cmake -S /home/m/src-cc3d/CompuCell3D/CompuCell3D -B /home/m/src-cc3d/CompuCell3D_gpu_
↪build -DPython3_EXECUTABLE=/home/m/miniconda3/envs/cc3d_gpu_compile/bin/python -DNO_
↪OPENCL=OFF  -DBUILD_STANDALONE=OFF -DOPENGL_gl_LIBRARY=/usr/lib/x86_64-linux-gnu/libGL.
↪so -DOPENGL_glx_LIBRARY=/usr/lib/x86_64-linux-gnu/libGLX.so -G "Unix Makefiles" -
↪DCMAKE_INSTALL_PREFIX=/home/m/src-cc3d/CompuCell3D_gpu_install
```

Here is the output of this command:

```
(cc3d_gpu_compile) m@m-lap:~/src-cc3d$ cmake -S /home/m/src-cc3d/CompuCell3D/CompuCell3D␣
↪-B /home/m/src-cc3d/CompuCell3D_gpu_build -DPython3_EXECUTABLE=/home/m/miniconda3/envs/
↪cc3d_gpu_compile/bin/python -DNO_OPENCL=OFF  -DBUILD_STANDALONE=OFF -DOPENGL_gl_
↪LIBRARY=/usr/lib/x86_64-linux-gnu/libGL.so -DOPENGL_glx_LIBRARY=/usr/lib/x86_64-linux-
↪gnu/libGLX.so -G "Unix Makefiles" -DCMAKE_INSTALL_PREFIX=/home/m/src-cc3d/CompuCell3D_
↪gpu_install -DOpenCL_LIBRARIES=/usr/lib/x86_64-linux-gnu/libnvidia-opencl.so.1
openmp c flags -fopenmp
openmp cxx flags -fopenmp
-- Found Python3: /home/m/miniconda3/envs/cc3d_gpu_compile/bin/python (found version "3.
↪10.0") found components: Interpreter Development NumPy Development.Module Development.
↪Embed
Python3_FOUND: TRUE
Python3_Interpreter_FOUND: TRUE
Python3_VERSION: 3.10.0
Python3_Development_FOUND: TRUE
Python3_EXECUTABLE: /home/m/miniconda3/envs/cc3d_gpu_compile/bin/python
Python3_Development_FOUND: TRUE
Python3_INCLUDE_DIRS: /home/m/miniconda3/envs/cc3d_gpu_compile/include/python3.10
Python3_LIBRARIES: /home/m/miniconda3/envs/cc3d_gpu_compile/lib/libpython3.10.so
Python3_LIBRARY_RELEASE: /home/m/miniconda3/envs/cc3d_gpu_compile/lib/libpython3.10.so
Python3_LIBRARY_DIRS: /home/m/miniconda3/envs/cc3d_gpu_compile/lib
Python3_RUNTIME_LIBRARY_DIRS: /home/m/miniconda3/envs/cc3d_gpu_compile/lib
Python3_NumPy_INCLUDE_DIRS: /home/m/miniconda3/envs/cc3d_gpu_compile/lib/python3.10/site-
↪packages/numpy/core/include
Python3_LIBRARY_DIRS /home/m/miniconda3/envs/cc3d_gpu_compile/lib
Python3_SABI_LIBRARY_DIRS
Python3_SITEARCH /home/m/miniconda3/envs/cc3d_gpu_compile/lib/python3.10/site-packages
PYTHON_BASE_DIR/home/m/miniconda3/envs/cc3d_gpu_compile
 THIS IS COMPUCELL3D_BUILD_VERSION 0
COMPUCELL3D_C_BUILD_VERSION is 0
GOT VERSION AS 4.6.0
 PUBLIC UTILS OPEN MP FLAG-fopenmp
expat library local /home/m/miniconda3/envs/cc3d_gpu_compile/lib/libexpat.so
-- /home/m/src-cc3d/CompuCell3D/CompuCell3D
CMake Warning (dev) at core/CompuCell3D/steppables/PDESolvers/FindEigen3.cmake:73:
  Syntax Warning in cmake code at column 35
```

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```
  Argument not separated from preceding token by whitespace.
Call Stack (most recent call first):
  core/CompuCell3D/steppables/PDESolvers/CMakeLists.txt:15 (find_package)
This warning is for project developers.  Use -Wno-dev to suppress it.

-- /home/m/src-cc3d/CompuCell3D/CompuCell3D/core/Eigen
-- Looking for OpenCL...
FOUND OPEN CL
-- OpenCL headers found at /home/m/miniconda3/envs/cc3d_gpu_compile/include
-- OpenCL library: /usr/local/cuda/lib64/libOpenCL.so
OPENMP FLAGS -fopenmp
-- Found Python3: /home/m/miniconda3/envs/cc3d_gpu_compile/bin/python (found suitable␣
↪version "3.10.0", minimum required is "3.10") found components: Interpreter␣
↪Development.Module Development.Embed
VTK_MAJOR_VERSION=9
NUMPY_INCLUDE_DIR
VTK_LIB_DIRS
THIS IS cc3d_py_source_dir: /home/m/src-cc3d/CompuCell3D/CompuCell3D/../cc3d
USING EXTERNAL PYTHON
-- Configuring done
CMake Warning (dev) at compucell3d_cmake_macros.cmake:200 (ADD_LIBRARY):
  Policy CMP0115 is not set: Source file extensions must be explicit.  Run
  "cmake --help-policy CMP0115" for policy details.  Use the cmake_policy
  command to set the policy and suppress this warning.

  File:

    /home/m/src-cc3d/CompuCell3D/CompuCell3D/core/CompuCell3D/steppables/PDESolvers/
↪hpppdesolvers.h
Call Stack (most recent call first):
  core/CompuCell3D/steppables/PDESolvers/CMakeLists.txt:187 (ADD_COMPUCELL3D_STEPPABLE)
This warning is for project developers.  Use -Wno-dev to suppress it.

-- Generating done
-- Build files have been written to: /home/m/src-cc3d/CompuCell3D_gpu_build
```

Note

It may happen that during cmake run command you may get an error about version of the Boost library (which VTK needs). In this case you should make a not of the Boost version that is suggested and install it int your environment. For example, if cmake output suggests to install boost version `1.85` we run the following

```
conda activate cc3d_gpu_compile
conda install -c conda-forge boost=1.85
```

and then repeat `cmake` command above.

If we look at the OpenCL section of the output:

```
FOUND OPEN CL
-- OpenCL headers found at /home/m/miniconda3/envs/cc3d_gpu_compile/include
-- OpenCL library: /usr/local/cuda/lib64/libOpenCL.so
```

We see that the correct OpenCL library was identified `/usr/local/cuda/lib64/libOpenCL.so`. If we look closed the `/usr/local/cuda/lib64/libOpenCL.so` is a soft-link to `/usr/local/cuda/lib64/libOpenCL.so`

```
(cc3d_gpu_compile) m@m-lap:~/src-cc3d$ ls -la /usr/local/cuda/lib64/libOpenCL.so
lrwxrwxrwx 1 root root 14 Apr 15 20:57 /usr/local/cuda/lib64/libOpenCL.so -> libOpenCL.
↪so.1
```

Once cmake prepares CC3D build we go to `/home/m/src-cc3d/CompuCell3D_gpu_build` - see last line of the cmake output:

```
-- Generating done
-- Build files have been written to: /home/m/src-cc3d/CompuCell3D_gpu_build
```

and run make and make install commands:

```
cd /home/m/src-cc3d/CompuCell3D_gpu_build
make -j 8
make install
```

at this point CC3D ith GPU solvers should be ready and if you want player just run

```
ln -s /home/m/src-cc3d/cc3d-player5/cc3d/player5   /home/m/miniconda3/envs/cc3d_gpu_
↪compile/lib/python3.10/site-packages/cc3d/player5
```

```
python -m cc3d.player
```

4.2.2 Benchmarking

When we run `SteppableDemos/DiffusionSolverFE_OpenCL/DiffusionSolverFE_OpenCL_3D/DiffusionSolverFE_OpenCL_3D.cc3d` project that uses GPU diffusion solver for 100 MCS here is the benchmarking report

```
           Total Steppable Time:        0.00 ( 0.0%)
Compiled Code (C++) Run Time:        1.44 (70.3%)
                  Other Time:        0.61 (29.6%)
```

Running the same simulation but without GPU acceleration gives the following runtime:

```
        Total Steppable Time:        0.00 ( 0.0%)
Compiled Code (C++) Run Time:       28.84 (98.0%)
                  Other Time:        0.60 ( 2.0%
```

As we can see we get approx 20x speedup for the diffusion constant of `1.0` . the speedups are greater for larger diffusion constants but in general the larger diffusion constant the longer the solver will run regardless if it is GPU or CPU solver

Even if we try using CPU multiprocessign by adding the following stub to `SteppableDemos/DiffusionSolverFE_OpenCL/DiffusionSolverFE_OpenCL_3D/DiffusionSolverFE_OpenCL_3D/DiffusionSolverFE_OpenCL_3D.xml`

```
 <Metadata>
   <NumberOfProcessors>16</NumberOfProcessors>
   <NonParallelModule Name="Potts"/>
</Metadata>
```

We still are getting slower performance that with the GPU but significantly faster than with just a single CPU:

```
        Total Steppable Time:        0.00 ( 0.0%)
Compiled Code (C++) Run Time:        6.39 (91.4%)
                  Other Time:        0.60 ( 8.6%)
```

In general, when benchmarking it is a good idea to keep those comparisons as fair as possible. We know that the power of GPU comes from many computational cores so, in that spirit, it seems fair to compare massively-multi-core GPU with multi-CPU implementation of a given algorithm - in this case the diffusion solver. As we have shown above, while GPU results in much shorter run-times than CPU, the performance gap can be narrowed by using multiple CPUs.

CHAPTER

FIVE

PREREQUISITES

We assume that you know C++ . To be more precise, you need to understand polymorphism, how virtual functions work and have basic knowledge of templates. We also assume that you are familiar with Cellular Potts Model, that is that you understand what CPM is all about and how it works. We will try to demonstrate how to develop new plugins by using a concrete example. This is probably the best way to introduce you to CompuCell3D development. Before we go there it is probably a good idea to understand how CompuCell3D works.

CHAPTER

SIX

POTTS3D

Potts3D module (`Potts3D/Potts3D.cpp`, `Potts3D/Potts3D.h`) implements entire logic of the Potts algorithm. In a nutshell Potts class contains implementation of a single Monte Carlo Step (MCS) of the Cellular Potts Model. The MCS works as follows:

1. Pick a random pixel from the lattice sites (call it source pixel)
2. Pick a neighboring pixel (based on user-defined neighborhood range) - let's call it change pixel
3. If the two pixels belong to different cells compute change in energy if we were to over change pixel with the cell currently occupying source pixel. This corresponds to the situation where the cell occupying change pixel would lose one pixel and cell occupying the source pixel would gain one pixel.
4. Compute acceptance probability of the proposed pixel copy
5. Perform pixel copy and update all cell attributes that change during such pixel copy. For example cell occupying source pixel increases its volume by 1 unit and cell occupying destination pixel decreases volume by one unit. Depending how you set up your simulation you would also update surface area of the tow cells, center of mass coordinates, intertia tensor etc.

Section *Implementing Cellular Potts Model in C++* covers in details the code that performs the tasks outlined above

Moreover, this module is responsible for creating cell lattice and `Potts3D` class has methods that facilitate creation and destruction of cells. It is worth pointing out that creation and destruction of cells is not limited to calling `new` or `delete` operators but it also involves several steps necessary to ensure that cells created have all the attributes needed by requested by the user plugins. In CC3D cells' attributes are added dynamically and CC3D cells by default have only a small subset of attributes hard-coded. This is a design decision that has this nice consequence that when developing new plugin one does not have to modify `CellG` class but rather program the addition of cell's attributes entirely in the plugins code. We will cover this in detail in later section.

Let's examine the content of the `Potts3D` class (**Note:** we removed some of the code and are presenting only code snippets most relevant to current discussion. You are encouraged to look at the original code though as you go over the material presented here):

```
class Potts3D :public SteerableObject {
        WatchableField3D<CellG *> *cellFieldG;
        AttributeAdder * attrAdder;
        EnergyFunctionCalculator * energyCalculator;

        BasicClassGroupFactory cellFactoryGroup;        //creates aggregate of objects␣
↪associated with cell


        /// An array of energy functions to be evaluated to determine energy costs.
        std::vector<EnergyFunction *> energyFunctions;
```

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```
        EnergyFunction * connectivityConstraint;

        std::map<std::string, EnergyFunction *> nameToEnergyFuctionMap;

...

        std::vector<BasicRandomNumberGeneratorNonStatic> randNSVec;

        /// An array of potts steppers.  These are called after each potts step.
        std::vector<Stepper *> steppers;

        std::vector<FixedStepper *> fixedSteppers;
        /// The automaton to use.  Assuming one automaton per simulation.
        Automaton* automaton;

...

        FluctuationAmplitudeFunction * fluctAmplFcn;

        /// The current total energy of the system.
        double energy;

        std::string boundary_x; // boundary condition for x axiz
        std::string boundary_y; // boundary condition for y axis
        std::string boundary_z; // boundary condition for z axis

        /// This object keeps track of all cells available in the simulations. It allows␣
↪for simple iteration over all the cells
        /// It becomes useful whenever one has to visit all the cells. Without inventory␣
↪one would need to go pixel-by-pixel - very inefficient
        CellInventory cellInventory;

        Point3D flipNeighbor;
        std::vector<Point3D> flipNeighborVec; //for parallel access

        double depth;
        //int maxNeighborOrder;
        std::vector<Point3D> neighbors;
        std::vector<unsigned char> frozenTypeVec;///lists types which will remain frozen␣
↪throughout the simulation
        unsigned int sizeFrozenTypeVec;

        ParallelUtilsOpenMP *pUtils;

public:

        Potts3D();
        Potts3D(const Dim3D dim);
        virtual ~Potts3D();

        void createCellField(const Dim3D dim);
        void resizeCellField(const Dim3D dim, Dim3D shiftVec = Dim3D());
```

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```
        double getTemperature() const { return temperature; }

        void registerConnectivityConstraint(EnergyFunction * _connectivityConstraint);
        EnergyFunction * getConnectivityConstraint();

        bool checkIfFrozen(unsigned char _type);

...

        void initializeCellTypeMotility(std::vector<CellTypeMotilityData> & _
↪cellTypeMotilityVector);
        void setCellTypeMotilityVec(std::vector<float> & _cellTypeMotilityVec);
        const std::vector<float> & getCellTypeMotilityVec() const { return␣
↪cellTypeMotilityVec; }

        void setDebugOutputFrequency(unsigned int _freq) { debugOutputFrequency = _freq;␣
↪}
        void setSimulator(Simulator *_sim) { sim = _sim; }

...

        Point3D getFlipNeighbor();

...

        virtual void createEnergyFunction(std::string _energyFunctionType);
        EnergyFunctionCalculator * getEnergyFunctionCalculator() { return␣
↪energyCalculator; }

        CellInventory &getCellInventory() { return cellInventory; }

        void clean_cell_field(bool reset_cell_inventory = true);

        virtual void registerAttributeAdder(AttributeAdder * _attrAdder);
        virtual void registerEnergyFunction(EnergyFunction *function);
        virtual void registerEnergyFunctionWithName(EnergyFunction *_function,␣
↪std::string _functionName);
        virtual void unregisterEnergyFunction(std::string _functionName);

        /// Add the automaton.
        virtual void registerAutomaton(Automaton* autom);

        /// Return the automaton for this simulation.
        virtual Automaton* getAutomaton();
        void setParallelUtils(ParallelUtilsOpenMP *_pUtils) { pUtils = _pUtils; }

        virtual void setFluctuationAmplitudeFunctionByName(std::string _
↪fluctuationAmplitudeFunctionName);
        /// Add a cell field update watcher.

        /// registration of the BCG watcher
```

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```
        virtual void registerCellGChangeWatcher(CellGChangeWatcher *_watcher);

        /// Register accessor to a class with a cellGroupFactory. Accessor will access a␣
↪class which is a mamber of a BasicClassGroup
        virtual void registerClassAccessor(BasicClassAccessorBase *_accessor);

        /// Add a potts stepper to be called after each potts step.
        virtual void registerStepper(Stepper *stepper);
        virtual void registerFixedStepper(FixedStepper *fixedStepper, bool _front =␣
↪false);
        virtual void unregisterFixedStepper(FixedStepper *fixedStepper);

        double getEnergy();

        virtual CellG *createCellG(const Point3D pt, long _clusterId = -1);
        virtual CellG *createCellGSpecifiedIds(const Point3D pt, long _cellId, long _
↪clusterId = -1);
        virtual CellG *createCell(long _clusterId = -1);
        virtual CellG *createCellSpecifiedIds(long _cellId, long _clusterId = -1);

        virtual void destroyCellG(CellG * cell, bool _removeFromInventory = true);

        BasicClassGroupFactory * getCellFactoryGroupPtr() { return &cellFactoryGroup; };

        virtual unsigned int getNumCells() { return cellInventory.getCellInventorySize();
↪ }

        virtual double changeEnergy(Point3D pt, const CellG *newCell,const CellG␣
↪*oldCell);

        virtual unsigned int metropolis(const unsigned int steps,const double temp);

        typedef unsigned int (Potts3D::*metropolisFcnPtr_t)(const unsigned int, const␣
↪double);

        metropolisFcnPtr_t metropolisFcnPtr;

        unsigned int metropolisList(const unsigned int steps, const double temp);

        unsigned int metropolisFast(const unsigned int steps, const double temp);
        unsigned int metropolisBoundaryWalker(const unsigned int steps, const double␣
↪temp);
        void setMetropolisAlgorithm(std::string _algName);

        virtual Field3D<CellG *> *getCellFieldG() { return (Field3D<CellG *>␣
↪*)cellFieldG; }
        virtual Field3DImpl<CellG *> *getCellFieldGImpl() { return (Field3DImpl<CellG *>␣
↪*)cellFieldG; }

        //SteerableObject interface
        virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag = false);
        virtual std::string steerableName();
```

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```
        virtual void runSteppers();
        long getRecentlyCreatedClusterId() { return recentlyCreatedClusterId; }
        long getRecentlyCreatedCellId() { return recentlyCreatedCellId; }

};
```

Starting from the top of the file we notice that cell lattice (`WatchableField3D<CellG *> *cellFieldG;`) is owned by `Potts3D` and created by (`void createCellField(const Dim3D dim);`, `void resizeCellField(const Dim3D dim, Dim3D shiftVec = Dim3D());`).

The cell lattice is an instance of the `WatchableField3D` class (which strictly speaking is a template class). The cell lattice stores **pointers** to cell objects (type `CellG*`). This means that when a single cell single occupies several lattice sites we create one `CellG` object but store pointer to this object in all locations of `cellFieldG` that are assigned to this particular instance of `CellG` object. This way `CellG` objects do not get repeated for every pixel (this would cost too much memory) but rather are referenced from the cell lattice via pointers. The reason cell lattice field is called "Watchable" is because this class implements the observer design pattern. This means that any manipulation of the cell lattice (e.g. assigning cell to a given pixel) triggers calls to multiple registered observer objects that react to such change. For example, if I am extending a cell by assigning its pointer to the new lattice site one of the observer that will be called (we also refer to them as lattice monitors) is a module that tracks cell volume The cell that gains new pixel will get its `volume` attribute increased by 1 and the cell that loses one pixel will get its volume decreased by 1. Similarly we could have another observer that updates center of mass coordinates, or one that monitors inertia tensor. The nice thing about using `WatchableField3D` template is that all those observers are called automatically when change in the lattice takes place. Observers are called in the order in which they were registered. Note, this may or may not be the order in which they were declared in the CC3DCML. CC3D sometimes requires certain lattice monitors to be loaded and registered before others and this happens automatically in the CC3D code. Let's look at how `WatchableField3D` works in practice:

6.1 WatchableField3D

```
#ifndef WATCHABLEFIELD3D_H
#define WATCHABLEFIELD3D_H

#include <vector>

#include "Field3DImpl.h"
#include "Field3DChangeWatcher.h"

#include <CompuCell3D/CC3DExceptions.h>

namespace CompuCell3D {

    template<class T>
    class Field3DImpl;

    template<class T>
    class WatchableField3D : public Field3DImpl<T> {
        std::vector<Field3DChangeWatcher<T> *> changeWatchers;

    public:
        /**
         * @param dim The field dimensions
         * @param initialValue The initial value of all data elements in the field.
```

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```
         */
        WatchableField3D(const Dim3D dim, const T &initialValue) :
                Field3DImpl<T>(dim, initialValue) {}

        virtual ~WatchableField3D() {}

        virtual void addChangeWatcher(Field3DChangeWatcher<T> *watcher) {
            if (!watcher) throw CC3DException("addChangeWatcher() watcher cannot be NULL!
↪");
            changeWatchers.push_back(watcher);
        }

        virtual void set(const Point3D &pt, const T value) {
            T oldValue = Field3DImpl<T>::get(pt);
            Field3DImpl<T>::set(pt, value);

            for (unsigned int i = 0; i < changeWatchers.size(); i++)
                changeWatchers[i]->field3DChange(pt, value, oldValue);
        }

        virtual void set(const Point3D &pt, const Point3D &addPt, const T value) {
            T oldValue = Field3DImpl<T>::get(pt);
            Field3DImpl<T>::set(pt, value);

            for (unsigned int i = 0; i < changeWatchers.size(); i++) {
                changeWatchers[i]->field3DChange(pt, value, oldValue);
                changeWatchers[i]->field3DChange(pt, addPt, value, oldValue);
            }
        }
    };
};
#endif
```

The `WatchableField3D<T>` template class inherits from `Field3DImpl<T>` template. The actual memory allocation takes place in the `Field3DImpl<T>` but we will not worry about it here. It is sufficient to mention that `Field3DImpl<T>` is tha class that manages cell lattice memory. The important thing is to understand how this automatic calling of lattice monitors is implemented. The `WatchableField3D<T>` class has a container `std::vector<Field3DChangeWatcher<T> *> changeWatchers;` that stores pointers to lattice monitors. The lattice monitor object is a class that inherits `Field3DChangeWatcher<T>` class. In CC3D case `T` is set to `CellG*`. The `BasicArray` is a thin wrapper around `std::vector` class and it is one of the legacies of the early CC3D implementations. So `WatchableField3D<T>` class has a collection of objects that react to the changes in the cell lattice. How do they react? If we look at the implementation of `virtual void set(const Point3D &pt, const T value)` function that modifies the lattice we can see that this function fetches old value stored in the lattice at location indicated by `Point3D pt` - in the case of cell lattice this will be pointers currently stored at this location. It then assigns new value to the field (new `CellG` pointer) and then it calls all registered lattice monitors:

```
for (unsigned int i = 0; i < changeWatchers.getSize(); i++)
      changeWatchers[i]->field3DChange(pt, value, oldValue);
```

In particular each lattice monitor (here referred to as `changeWatcher`) must define function called `field3DChange` that takes 3 arguments - location of the change `pt`, new value we assign to the field (e.g. new pointer to `CellG` object) and old value that was stored in the field before the assignment (e.g. pointer to the cell whose pixel gets overwritten).

This way the process of updating attributes of `CellG` object can be handled by appropriate `changeWatchers`. We will cover in detail examples of change watchers and things will become clearer then.

6.2 Energy Functions

Few lines below declaration of `cellField`, which as we know is an instance of `WatchableField3D<CellG *>` we find the declaration of containers associated with Energy function calculations. At this point we remind that the essence of Cellular Potts Model is in calculating **change of energy of the system due to randomly chosen lattice perturbation** (change of the single pixel). Pointers to energy functions objects are stored inside `Potts3D` object as follows:

```
/// An array of energy functions to be evaluated to determine energy costs.
std::vector<EnergyFunction *> energyFunctions;
EnergyFunction * connectivityConstraint;

std::map<std::string, EnergyFunction *> nameToEnergyFuctionMap;
```

All energy functions are actually objects and they all inherit base class `EnergyFunction`. `EnergyFunction` is defined inside `Potts3D/EnergyFunction.h` header file:

```
class EnergyFunction {

public:
        EnergyFunction() {}
        virtual ~EnergyFunction() {}

        virtual double localEnergy(const Point3D &pt){return 0.0;};

        virtual double changeEnergy(const Point3D &pt, const CellG *newCell,const CellG␣
↪*oldCell)
        {
                if(1!=1);return 0.0;
        }
        virtual std::string toString()
        {
                return std::string("EnergyFunction");
        }
};
```

Each class that is responsible for calculating a **change in the overall system energy due to a proposed pixel copy** has to inherit `EnergyFunction`. The key function that has to be reimplemented in the derived class is `virtual double changeEnergy(const Point3D &pt, const CellG *newCell,const CellG *oldCell)`. After Metropolis algorithm function picks candidate for pixel overwrite it will then call `changeEnergy` for every element of the `energyFunctions` vector defined in class `Potts3D` (see above). The `pt` argument is a reference to a location of a pixel (specified as simple object `Point3D`) that would be overwritten as result of the pixel copy attempt. The `newCell` is pointer to a cell object that will occupy `pt` location of the `cellField` (if we accept pixel copy) and the `oldCell` is a pointer to a cell that currently occupies lattice location `pt`.

In CompuCell3D users declare which energy functions they want to use in their simulation so that the number of energy function in the `energyFunctions` vector will vary depending on what users specify in the CC3DML or in Python.

Later we will present detailed information on how to implement energy function plugins.

6.2.1 Implementing Cellular Potts Model in C++ - metropolisFast method

When we peek at the `metropolisFast` function of the `Potts3D` class we can see that the change of energy is calculated in a fairly straightforward way:

```
Point3D pt;

// Pick a random point
pt.x = rand->getInteger(sectionDims.first.x, sectionDims.second.x - 1);
pt.y = rand->getInteger(sectionDims.first.y, sectionDims.second.y - 1);
pt.z = rand->getInteger(sectionDims.first.z, sectionDims.second.z - 1);

CellG *cell = cellFieldG->getQuick(pt);

if (sizeFrozenTypeVec && cell) {///must also make sure that cell ptr is different 0;␣
↪Will never freeze medium
    if (checkIfFrozen(cell->type))
        continue;
}

unsigned int directIdx = rand->getInteger(0, maxNeighborIndex);

Neighbor n = boundaryStrategy->getNeighborDirect(pt, directIdx);

if (!n.distance) {
    //if distance is 0 then the neighbor returned is invalid
    continue;
}
Point3D changePixel = n.pt;

//check if changePixel refers to different cell.
CellG* changePixelCell = cellFieldG->getQuick(changePixel);

if (changePixelCell == cell) {
    //skip the rest of the loop if change pixel points to the same cell as pt
    continue;
}

if (sizeFrozenTypeVec && changePixelCell) {///must also make sure that cell ptr is␣
↪different 0; Will never freeze medium
    if (checkIfFrozen(changePixelCell->type))
        continue;
}

++attemptedECVec[currentWorkNodeNumber];

flipNeighborVec[currentWorkNodeNumber] = pt;

/// change takes place at change pixel  and pt is a neighbor of changePixel
// Calculate change in energy

double change = energyCalculator->changeEnergy(changePixel, cell, changePixelCell, i);
```

We first pick a random lattice location `pt` and retrieve pointer of a cell that occupies this location:

```
CellG *cell = cellFieldG->getQuick(pt);
```

We next make sure that the cell can move *i.e.* it is not frozen:

```
if (sizeFrozenTypeVec && cell) {///must also make sure that cell ptr is different 0;␣
↪Will never freeze medium
    if (checkIfFrozen(cell->type))
        continue;
}
```

Next we pick a random pixel out of set of neighbors of pixel `pt`:

```
unsigned int directIdx = rand->getInteger(0, maxNeighborIndex);

Neighbor n = boundaryStrategy->getNeighborDirect(pt, directIdx);

if (!n.distance) {
    //if distance is 0 then the neighbor returned is invalid
    continue;
}
Point3D changePixel = n.pt;

//check if changePixel refers to different cell.
CellG* changePixelCell = cellFieldG->getQuick(changePixel);

if (changePixelCell == cell) {
    //skip the rest of the loop if change pixel points to the same cell as pt
    continue;
}

if (sizeFrozenTypeVec && changePixelCell) {///must also make sure that cell ptr is␣
↪different 0; Will never freeze medium
    if (checkIfFrozen(changePixelCell->type))
        continue;
}
```

We use `BoundaryStrategy` object pointed by `boundaryStrategy` to carry out all operations related to pixel neighbor operations. we will cover it later. For now it is important to remember that tracking and operating on pixel neighbors is usually done via `BoundaryStrategy` and this helps greatly when we have to deal with periodic boundary conditions pixels residing close to the edge of the lattice or classifying neighbor order of pixels. In this example we use boundary strategy to pick a neighbor `changePixel` of the `pt` and verify that this neighbor is a legitimate neighbor - `if (!n.distance)`. We next fetch cell that occupies `changePixel`:

```
CellG* changePixelCell = cellFieldG->getQuick(changePixel);
```

and verify that `changePixelCell` is different than cell at the location `pt`. We do this because overwriting pixel with the same cell pointer does not change lattice configuration at all. After also confirming that the `changePixelCell` is not frozen we compute change of energy if pixel `changePixel` currently occupied by `changePixelCell` were to be overwritten by `cell` currently residing at location `pt`. Or using `double changeEnergy(const Point3D &pt, const CellG *newCell,const CellG *oldCell)` terminology we can say that `pt <-> changePixel`, `newCell <-> cell` and `oldCell <-> changePixelCell` where we used <-> symbol to illustrate how `changeEnergy` function arguments will be assigned in the call.

Interestingly, we call `changeEnergy` method of the object called `energyCalculator`:

```
double change = energyCalculator->changeEnergy(changePixel, cell, changePixelCell, i);
```

There is no magic here. If we look inside this function (`Potts3D/EnergyFunctionCalculator.cpp`) we see familiar summation over all values returned by `changeEnergy` of each `EnergyFunction` object:

```
double EnergyFunctionCalculator::changeEnergy(Point3D &pt, const CellG *newCell,const␣
↪CellG *oldCell,const unsigned int _flipAttempt){

    double change = 0;
    for (unsigned int i = 0; i < energyFunctions.size(); i++){
        change += energyFunctions[i]->changeEnergy(pt, newCell, oldCell);
    }
    return change;
}
```

The reason we use `EnergyFunctionCalculator` object instead of implementing summation loop inside `metropolisFast` function is to handle additional tasks that might be associated with calculating energies - for example collecting information on every energy term associated with every pixel copy attempts. In this case we would use not `EnergyFunctionCalculator` but a more sophisticated version of this class called `EnergyFunctionCalculatorStatistics`

6.3 Steppers

A vector of `Stepper` objects - `std::vector<Stepper *> steppers;` is also a part of `Potts3D` object. Stepper objects all inherit from `Stepper` class defined in `Potts3D/Stepper.h` header file:

```
class Stepper {
public:
    virtual void step() = 0;
};
```

This is a very simple base class that defines only one function called `step`. More important is the question where and **why** we need this function. Steppers are called at the very end of the pixel copy attempt *i.e.* after all energy function calculation and if pixel copy was accepted after modifying `cellField`. Steppers are called always regardless whether pixel copy was accepted or not. A canonical example of the `Stepper` object is `VolumeTracker` declared and defined in `plugins/VolumeTracker/VolumeTrackerPlugin.h` and `plugins/VolumeTracker/VolumeTrackerPlugin.cpp`. `VolumeTracker` plugin tracks volume of each cell and ensures that cells' volume information is correct. It also removes dead cells i./e. those cells whose volume reached 0. In a sense it performs cleanup actions. However cleanup needs to be done as a very last action associated with pixel copy attempt. It would be a bad idea to do it earlier because we could remove cell object that might still be needed by other actions related to *e.g.* updating `cellField`.

6.4 Cell Inventory

`cellInventory` as its name suggest is an object that serves as a container for pointers to cell objects but it also allows fast lookups of particular cells. This is one of he most frequently accessed objects from Python (although we do it somewhat indirectly). Many of the Python modules you write for CC3D include the following loop:

```
for cell in self.cell_list:
    ...
```

What we are doing here is we iterate over every cell in the simulation. Internally the `self.cell_list` Python object accesses `cellInventory`. when we create a cell using `Potts3D`'s method `createCellG` we first construct cell object and then insert it into cell inventory. Similarly when we delete cell object using `destroyCellG` (method of `Potts3D`)

we first remove the `cell` object from inventory and then carryout its destruction (which, as you know, is not just simple call to the C++ `delete` operator). It is worth knowing that in addition to cell inventories e track cell clusters and even links between cells (`FocalPointPlasticityPlugin`) via various "inventory" objects.

6.5 Acceptance Function and Fluctuation Amplitude Function

A key component of the Cellular Potts Model simulation is the so called acceptance function. It is the function that is responsible for they dynamic behavior of the simulation. It takes as an input a change in energy due to proposed pixel copy and outputs a probability with which this proposed pixel copy attempt will be accepted

Canonical formulation of the Cellular Potts Model acceptance function is as follows:
$$\begin{cases} P = e^{-(\Delta E - \delta)/kT} \text{ if } \Delta E > 0 \\ 1 \text{ if } \Delta E > 0 \\ 1/2 \text{ if } \Delta E = 0 \end{cases}$$
where ΔE is a change in the energy due to proposed pixel copy attempt T is the the "temperature" which is a measure of cell membrane fluctuation amplitude and k is a constant which by default is set to `1` and δ is an energy offset by default set to `0`

The higher the `T` is the higher the chance of accepting pixel copy attempts that result in higher energy Those appear to be the "wrong" kind of attempts but it turns out that they often save the simulation from being stuck in a local minimum so ensuring some of them are accepted is essential.

The "temperature" or membrane fluctuation amplitude parameter can be set globally and many of the simulations using this convention. However, you can imagine that certain cells may have different membrane fluctuation amplitudes (different "temperatures"). To account for this fact and the fact that the two cells involved in pixel copy attempt may have different "temperatures" we use objects that derive from `FluctuationAmplitudeFunction` and whose goal is to compute effective "temperature" parameter associated with pixel copy based on the two "temperature" parameters that come from two cells involved in pixel copy. There are many possibilities here but the default strategy is to choose minimum of the two "temperatures". The details can be found in `Potts3D/StandardFluctuationAmplitudeFunctions.h` and `Potts3D/StandardFluctuationAmplitudeFunctions.cpp`. We can also create new fluctuation amplitude functions depending on our needs.

CHAPTER

SEVEN

SIMULATOR

`Simulator` is the key C++ module that sits at the root of each simulation run by CC3D. This is essentially a single class `Simulator` and it is responsible for orchestrating the flow of each CC3D simulation. Simulator object creates and manages other key objects such as `Potts3D` and ensures the integrity of the entire simulation. The code for the object is stored in `CompuCell3D\Simulator.h` and `CompuCell3D\Simulator.cpp`. If there is one thing to remember about the Simulator object is that it interchangeably calls function from Potts that implements MOnt Carlo Step (e.g. `metropolisFast` function) followed by call to all steppables (modules that are called after each Monte Carlo Step)

Let us look at the header file of the `Simulator` to examine the responsibilities that `Simulator` when running CC3D simulations

```
namespace CompuCell3D {
    class ClassRegistry;
    class BoundaryStrategy;

    template <typename Y> class Field3DImpl;
    class Serializer;
    class PottsParseData;
    class ParallelUtilsOpenMP;

    class COMPUCELLLIB_EXPORT Simulator : public Steppable {

        ClassRegistry *classRegistry;

        Potts3D potts;

        int currstep;

        bool simulatorIsStepping;
        bool readPottsSectionFromXML;
        std::map<std::string,Field3D<float>*> concentrationFieldNameMap;
        //map of steerable objects
        std::map<std::string,SteerableObject *> steerableObjectMap;

        std::vector<Serializer*> serializerVec;
        std::string recentErrorMessage;
        bool newPlayerFlag;

        std::streambuf * cerrStreamBufOrig;
        std::streambuf * coutStreamBufOrig;
        CustomStreamBufferBase * qStreambufPtr;
```

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```
        std::string basePath;
        bool restartEnabled;

    public:

        ParserStorage ps;
        PottsParseData * ppdCC3DPtr;
        PottsParseData ppd;
        PottsParseData *ppdPtr;
        ParallelUtilsOpenMP *pUtils;
        ParallelUtilsOpenMP *pUtilsSingle; // stores same information as pUtils but␣
↪assumes that we use only single CPU - used in modules for which user requests single␣
↪CPU runs e.g. Potts with large cells

        double simValue;

        void setOutputRedirectionTarget(ptrdiff_t  _ptr);
        ptrdiff_t getCerrStreamBufOrig();
        void restoreCerrStreamBufOrig(ptrdiff_t _ptr);

        void setRestartEnabled(bool _restartEnabled){restartEnabled=_restartEnabled;}
        bool getRestartEnabled(){return restartEnabled;}

        static PluginManager<Plugin> pluginManager;
        static PluginManager<Steppable> steppableManager;
        static BasicPluginManager<PluginBase> pluginBaseManager;
        Simulator();
        virtual ~Simulator();
        //     PluginManager::plugins_t & getPluginMap(){return pluginManager.
↪getPluginMap();}

        //Error handling functions
        std::string getRecentErrorMessage(){return recentErrorMessage;}
        void setNewPlayerFlag(bool _flag){newPlayerFlag=_flag;}
        bool getNewPlayerFlag(){return newPlayerFlag;}

        std::string getBasePath(){return basePath;}
        void setBasePath(std::string _bp){basePath=_bp;}

        ParallelUtilsOpenMP * getParallelUtils(){return pUtils;}
        ParallelUtilsOpenMP * getParallelUtilsSingleThread(){return pUtilsSingle;}

        BoundaryStrategy * getBoundaryStrategy();
        void registerSteerableObject(SteerableObject *);
        void unregisterSteerableObject(const std::string & );
        SteerableObject * getSteerableObject(const std::string & _objectName);

        void setNumSteps(unsigned int _numSteps){ppdCC3DPtr->numSteps=_numSteps;}
        unsigned int getNumSteps() {return ppdCC3DPtr->numSteps;}
        int getStep() {return currstep;}
        void setStep(int currstep) { this->currstep = currstep; }
        bool isStepping(){return simulatorIsStepping;}
```

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```
        double getFlip2DimRatio(){return ppdCC3DPtr->flip2DimRatio;}
        Potts3D *getPotts() {return &potts;}
        Simulator *getSimulatorPtr(){return this;}
        ClassRegistry *getClassRegistry() {return classRegistry;}

        void registerConcentrationField(std::string _name,Field3D<float>* _fieldPtr);
        std::map<std::string,Field3D<float>*> & getConcentrationFieldNameMap(){
            return concentrationFieldNameMap;
        }
        void postEvent(CC3DEvent & _ev);

        std::vector<std::string> getConcentrationFieldNameVector();
        Field3D<float>* getConcentrationFieldByName(std::string _fieldName);

        void registerSerializer(Serializer * _serializerPtr){serializerVec.push_back(_
↪serializerPtr);}
        virtual void serialize();

        // Begin Steppable interface
        virtual void start();
        virtual void extraInit();///initialize plugins after all steppables have been␣
↪initialized
        virtual void step(const unsigned int currentStep);
        virtual void finish();
        // End Steppable interface

        //these two functions are necessary to implement proper cleanup after the␣
↪simulation
        //1. First it cleans cell inventory, deallocating all dynamic attributes - this␣
↪has to be done before unloading modules
        //2. It unloads dynamic CC3D modules - plugins and steppables
        void cleanAfterSimulation();
        //unloads all the plugins - plugin destructors are called
        void unloadModules();

        void initializePottsCC3D(CC3DXMLElement * _xmlData);
        void processMetadataCC3D(CC3DXMLElement * _xmlData);

        void initializeCC3D();
        void setPottsParseData(PottsParseData * _ppdPtr){ppdPtr=_ppdPtr;}
        CC3DXMLElement * getCC3DModuleData(std::string _moduleType,std::string _
↪moduleName="");
        void updateCC3DModule(CC3DXMLElement *_element);
        void steer();

    };
};
```

Few things to notice:

1. All CompuCell3D classes are defined within `CompuCell3D` namespace:

```
namespace CompuCell3D {
    class ClassRegistry;
    ...
    class COMPUCELLLIB_EXPORT Simulator : public Steppable {
    ...
    };
};
```

2. Most CC3D objects are dynamically loaded. To make sure an object can be dynamically loaded on Windows we need to include `__decl(dllimport)` and `__decl(dllexport)` class decorators as introduced and required by Microsoft Visual Studio Compilers. Therefore the C++ macro you see above -`COMPUCELLLIB_EXPORT` contains required decorators on Windows and is an empty string on all other operating systems. You can find the details of the Microsoft decorators here:

- https://stackoverflow.com/questions/14980649/macro-for-dllexport-dllimport-switch

3. `Simulator` contains `Potts3D` object :

```
namespace CompuCell3D {
    class ClassRegistry;
    ...
    class COMPUCELLLIB_EXPORT Simulator : public Steppable {
        ClassRegistry *classRegistry;

        Potts3D potts;
    ...
    };
};
```

4. `Simulator` has dictionary of every concentration field used in the simulation

```
std::map<std::string,Field3D<float>*> concentrationFieldNameMap;
```

Those fields can be accessed by external code (e.g. Plugin or Steppable code) by using the following `Simulator` methods:

```
std::vector<std::string> getConcentrationFieldNameVector();
Field3D<float>* getConcentrationFieldByName(std::string _fieldName);
```

where `getConcentrationFieldNameVector()` retrieves a vector of names of the fields used in the simulation and `Field3D<float>* getConcentrationFieldByName(std::string _fieldName)` returns a pointer to a field

5. Functions/class members related to streams *e.g.* `std::streambuf * cerrStreamBufOrig;` are related to redirecting output to either console or to a GUI. We will not discuss them here

6. Core simulator functionality, as far as the flow of the simulation is concerned, is implemented in the following functions:

```
void initializeCC3D();
virtual void start();
virtual void extraInit();///initialize plugins after all steppables have been initialized
virtual void step(const unsigned int currentStep);
virtual void finish();
```

- `void initializeCC3D()` initializes `Potts3D` object based on the CC3DML content , as well as loadable modules such as Plugins and Steppables and it is the first Simulator function that is called after parsing of the

CC3DML is complete

- `void extraInit()` is typically executed next and it calls `extraInit` method that is a member of every CompuCell3D plugin. Think of this function as a way of performing a second round of initialization but in the situation where all necessary objects (plugins) are instantiated and properly located inside overseeing objects (`Simulator` / `Potts3D`)
- `void start()` function calls `start` method for all Steppables that were requested by current simulation.
- `void step(const unsigned int currentStep)` method executes a single Monte Carlo Step (**MCS**) by calling `metropolis` method from Potts3D;

```
int flips = potts.metropolis(flipAttempts, ppdCC3DPtr->temperature);
```

and it also calls `step` method of every steppable requested by the simulation (including PDE solvers) by calling `step` method of a `classRegistry` member of the `Simulator` object. You may think about `classRegistry` as of a container that stores pointers to Steppable objects. Indeed, if we looks a the `CompuCell3D\ClassRegistry.h` declarations we notice that `ClassRegistry` class is a collection of containers with extra functionality that simplify code calls from parent objects (*e.g.* from `Simulator`):

```
namespace CompuCell3D {
  class Simulator;

  class COMPUCELLLIB_EXPORT ClassRegistry : public Steppable {
    BasicClassRegistry<Steppable> steppableRegistry;

    typedef std::list<Steppable *> ActiveSteppers_t;
    ActiveSteppers_t activeSteppers;

    typedef std::map<std::string, Steppable *> ActiveSteppersMap_t;
    ActiveSteppersMap_t activeSteppersMap;

    Simulator *simulator;

    std::vector<ParseData *> steppableParseDataVector;

  public:
    ClassRegistry(Simulator *simulator);
    virtual ~ClassRegistry() {}

    Steppable *getStepper(std::string id);

     void addStepper(std::string _type, Steppable *_steppable);

    // Begin Steppable interface
    virtual void extraInit(Simulator *simulator);
    virtual void start();
    virtual void step(const unsigned int currentStep);
    virtual void finish();
    // End Steppable interface

    virtual void initModules(Simulator *_sim);
  };
};
```

- Finally the `void finish()` method is responsible finishing the simulation. This seemingly simple task involves

few critical steps: running few Monte Carlo Steps (of metropolis algorithm) with zero temperature - users specify number of those steps in the CC3DML code (in <Anneal> element), calling `finish` function of every steppable, unloading dynamically loaded modules (Plugins and Steppables) to ensure that subsequent simulations can run without restarting CC3D.

There are clearly more methods in the Simulator objects but the ones described perform most of the work.

CHAPTER

EIGHT

DEVELOPING CC3D C++ MODULES

In this and following sections we will teach you how to develop core CC3D modules. In a typical scenario modelers might be interested in developing 3 types of modules:

1. Steppables - those are the modules that Simulator calls after each MCS. Examples include e.g. PDE solvers. THose modules are the most intuitive to write because typically you either visit all cells in the simulation or all lattice pixels and perform required operations.
2. Lattice Monitors - this are the modules that are called each time CC3D functions e.g. `metropolisFast` makes a change to the cell lattice. The simples example would be volume tracker - a module responsible for incrementing the volume of the cell that extends its set of pixels due to pixel copy and decrementing the volume of th cell that loses single pixe due to pixel copy.
3. Energy Function - this module is called every pixel copy attempt because Potts algorithm calls this module to compute its contribution to the overall change of energy due to proposed pixel copy.

The above modules are ranked in increasing c all frequency with energy functions being called the most frequently followed by lattice monitors and steppables.

To begin developing CC3D modules make sure you have installation of CC3D on your computer. Next you need to install `git` repository management software and after this you would clone a CC3D repository into your local hard drive:

THe following commands work on Unix systems but you can easily modify them to work on Windows as well.

```
mkdir -p ~/src-cc3d/
cd ~/src-cc3d/
git clone https://github.com/CompuCell3D/CompuCell3D.git
```

Here we created `src-cc3d` folder in the home directory and cloned CC3D repository there. You should see `~/src-cc3d/CompuCell3D` on your hard-drive.

CHAPTER

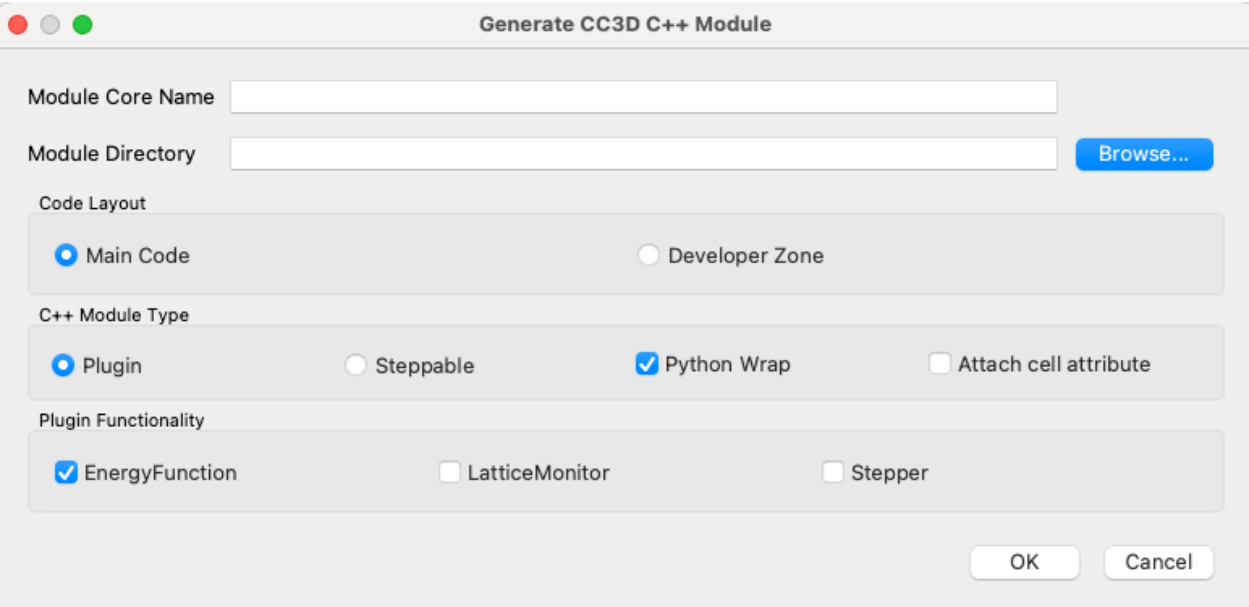
NINE

SIMPLE VOLUME TRACKER IN C++

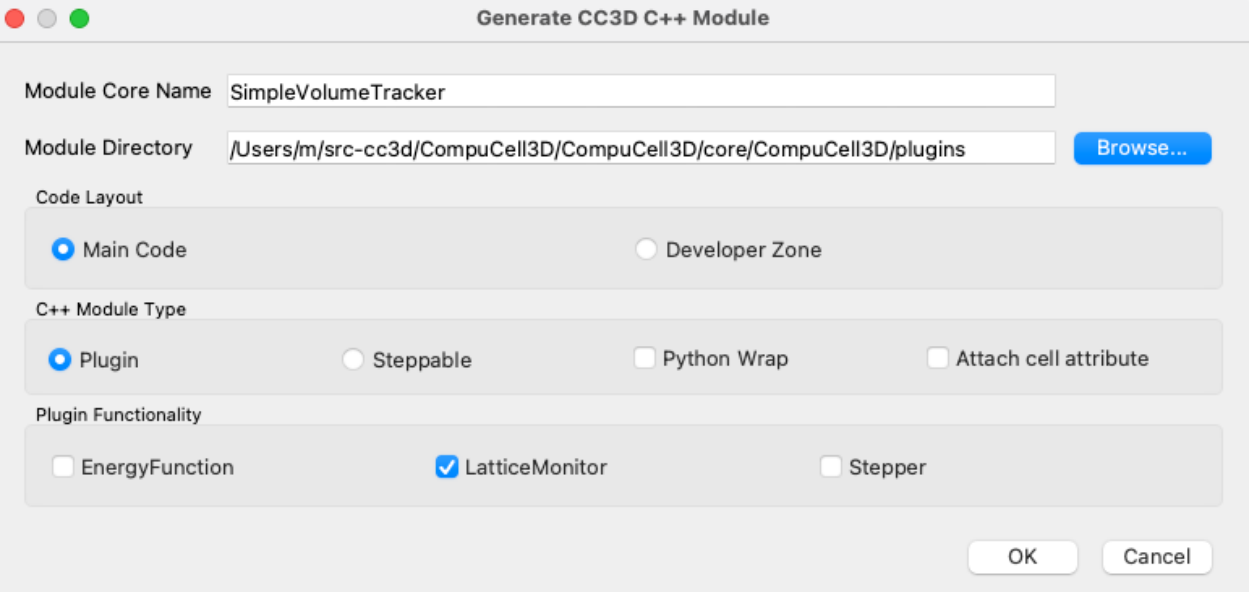
The purpose of this tutorial is to show you a simplified version of the real Volume Tracker that is implemented in the CompuCell3D. We will guide you step by step how to develop the code. ANd later show you how to compile it and how to use it in a simulation. Note that this will be rather a toy module because real VolumeTracker is loaded with every simulation we cannot have two modules incrementing and decrementing volumes . our version will only do printouts each time the cell's volume is incremented or decremented. The reason we begin with this toy example is because it is probably the simples lattice monitor plugin one can write.

We assume that you cloned CompuCell3D repository to `~/src-cc3d/CompuCell3D`

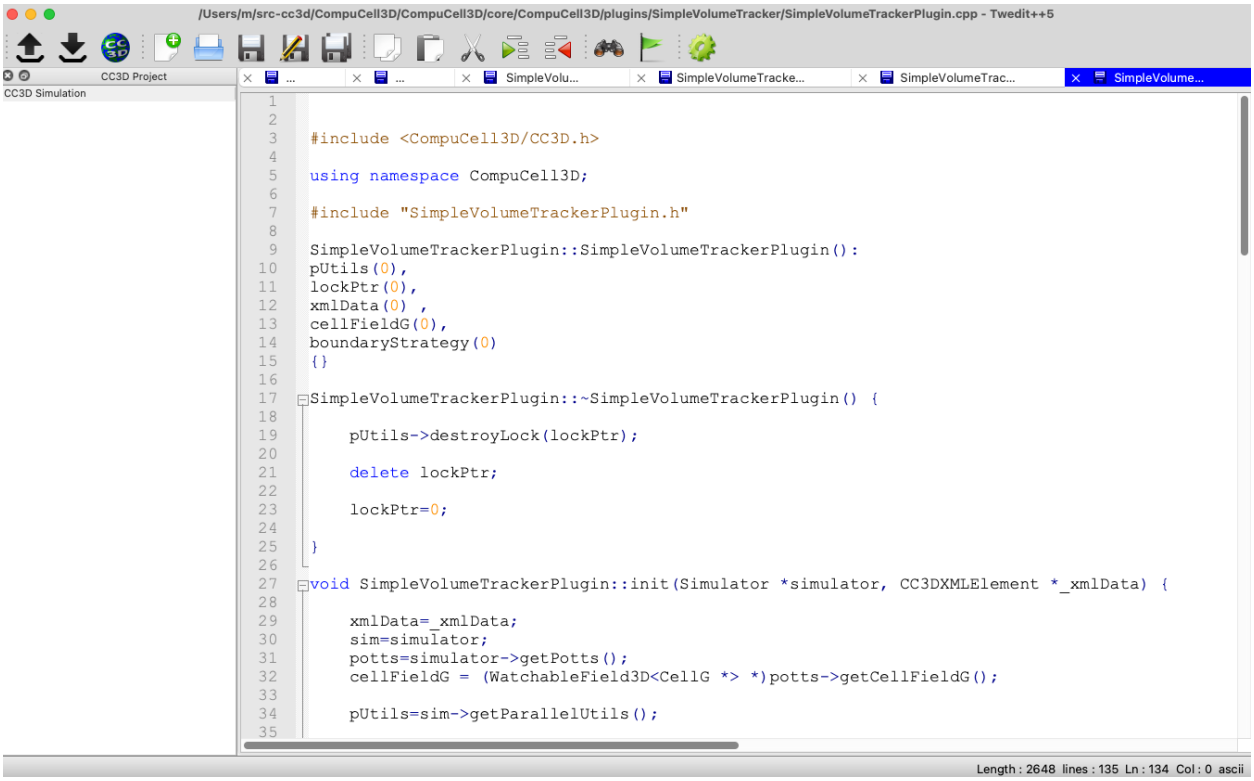
To begin, lets launch Twedit++. Then from CC3D C++ Menu lets select `Generate New Module...` and you should see the dialog:



We need to fill module name, point to the directory where the code should be generated and select if the code should be generated in Developer Zone or in the main code layout. We will pick main layout, call module `SimpleVolumeTracker` and pick `/Users/m/src-cc3d/CompuCell3D/CompuCell3D/core/CompuCell3D/plugins` as a module directory. The Module Type is `Plugin` and we pick `LatticeMonitor` as a Plugin functionality



After, we click OK Twedit++ will generate code template that compiles out-of-the-box but does nothing interesting. The important thing is that Twedit++ generates a lot of boiler-plate code that we would need to write manually. This is a very tedious task and by using Twedit++ we saved ourselves a lot of work.



It is our task to make this code useful. We will do it now. Here is the template of the core function (`field3DChange`) that Each Lattice Monitor needs to implement.

```
void SimpleVolumeTrackerPlugin::field3DChange(const Point3D &pt, CellG *newCell, CellG␣
↪*oldCell)
```

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```
{
    //This function will be called after each successful pixel copy - field3DChange does␣
↪usual housekeeping tasks to make sure state of cells, and state of the lattice is␣
↪update

    if (newCell){
        //PUT YOUR CODE HERE
    }else{
        //PUT YOUR CODE HERE
    }

    if (oldCell){
        //PUT YOUR CODE HERE
    }else{
        //PUT YOUR CODE HERE
    }
}
```

Here is how we can modify it:

```
void SimpleVolumeTrackerPlugin::field3DChange(const Point3D &pt, CellG *newCell, CellG␣
↪*oldCell)

{
    //This function will be called after each successful pixel copy - field3DChange does␣
↪usual housekeeping tasks to make sure state of cells, and state of the lattice is␣
↪update

    if (newCell){
        cerr<<"Cell id "<<newCell->id<<" increases volume by 1"<<endl;
    }else{
        cerr<<"Medium - source cell overwrites another cell's voxel"<<endl;
    }

    if (oldCell){
        cerr<<"Cell id "<<oldCell->id<<" decreases volume by 1"<<endl;
    }else{
        cerr<<"Medium - target cell's voxel gets overwritten by another cell"<<endl;
    }
}
```

Here is how this code works:

1) `field3DChange` will be called after `newCell` overwrites pixel occupied by the `oldCell`. This call is triggered automatically from the `metropolisFast` function. How does metropolisFast know which lattice monitory to call - we will cover it soon.

2) It may happen that pointer to `newCell` or `oldCell` may be NULL which corresponds to situation where either of these cells is Medium. We need to handle this case so that we do not attempt to access `id` or `volume` attribute of the NULL pointer.

3) Since `newCell` is the cell that overwrites another cell - it is the cell whose volume increases. By analogy, oldCell is the one that is overwritten, hence loses one pixel.

4) the else portion of the code handles situation where we are dealing with Medium. Medium is represented in

CC3D as a `null` pointer and hence we need to handle it as such

Let us compile the project. Since we have already did our initial setup involving cmake all we need to do is to run `make` and `make install`

```
cd /Users/m/src-cc3d/CompuCell3D_build
make -j 8
make install
```

This next step is only required if we modified core CC3D files like Potts.cpp or Simulator.cpp If we worked on plugin code only we can skip it

```
cp /Users/m/src-cc3d/CompuCell3D_install/lib/*.dylib /Users/m/miniconda3_arm64/envs/cc3d_
↪compile/lib
```

Note

Notice that if we did any modification to `CMakeLists.txt` files (and Twedit++ did ir for us during plugin code generation) the first thing that happens when we run `make` command is reconfiguration of the entire cmake Build system but fortunately thi sis done automatically. We only need to call cmake command once , when we first det up the compilation of CompuCell3D. The only downside on Mac is that this reconfiguration of the cmake build system for our compilation directory of CC3D will cause recompilation of the entire CompuCell3D. However, this will only happen if add new module or modify CmakeLists.txt files. If we change the C++ code for the plugin only the plugin should get compiled

After we compile this plugin (see materials on how to compile CC3D on your platform) we can use it in our simulation. Insert the following

```
<Plugin Name="SimpleVolumeTracker"/>
```

inside XML - in my case `/Users/m/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/cellsort/cellsort_2D/Simulation/cellsort_2D.xml`:

```
<CompuCell3D>
    <Potts>
        <Dimensions x="100" y="100" z="1"/>
        <Anneal>10</Anneal>
        <Steps>10000</Steps>
        <Temperature>10</Temperature>
        <Flip2DimRatio>1</Flip2DimRatio>
        <NeighborOrder>2</NeighborOrder>
    </Potts>


    <Plugin Name="Volume">
        <TargetVolume>25</TargetVolume>
        <LambdaVolume>2.0</LambdaVolume>
    </Plugin>

    <Plugin Name="CellType">
        <CellType TypeName="Medium" TypeId="0"/>
        <CellType TypeName="Condensing" TypeId="1"/>
        <CellType TypeName="NonCondensing" TypeId="2"/>
```

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```
    </Plugin>

    <Plugin Name="Contact">
        <Energy Type1="Medium" Type2="Medium">0</Energy>
        <Energy Type1="NonCondensing" Type2="NonCondensing">16</Energy>
        <Energy Type1="Condensing" Type2="Condensing">2</Energy>
        <Energy Type1="NonCondensing" Type2="Condensing">11</Energy>
        <Energy Type1="NonCondensing" Type2="Medium">16</Energy>
        <Energy Type1="Condensing" Type2="Medium">16</Energy>
        <NeighborOrder>2</NeighborOrder>
    </Plugin>

    <Plugin Name="SimpleVolumeTracker"/>

    <Steppable Type="BlobInitializer">

        <Region>
            <Center x="50" y="50" z="0"/>
            <Radius>40</Radius>
            <Gap>0</Gap>
            <Width>5</Width>
            <Types>Condensing,NonCondensing</Types>
        </Region>
    </Steppable>


</CompuCell3D>


then run it using
```

```
python -m cc3d.run_script -i /Users/m/src-cc3d/CompuCell3D/CompuCell3D/core/Demos/Models/
↪cellsort/cellsort_2D/cellsort_2D.cc3d
```

and we should get printouts printouts that look as follows:

```
Cell id 148 decreases volume by 1
Cell id 149 increases volume by 1
Cell id 162 decreases volume by 1
Cell id 83 increases volume by 1
Cell id 82 decreases volume by 1
Cell id 189 increases volume by 1
Cell id 188 decreases volume by 1
```

Congratulations. You have developed your first CompuCell3D plugins. Even though the SimpleVolumeTracker in its current form is not terribly useful it taught us the mechanics of adding new plugin, compiling cc3d and using new plugin with freshly compiled CC3D. In the next chapters we will develop more pragmatic examples

CHAPTER

TEN

SIMPLE VOLUME TRACKER IN C++ PART 2 - CHANGING CELL TYPE

Our previous example showed us how to do printouts from our newly written plugin. Now lets write code that alters cell state. We will implemement functionality that if any cell in simulation reaches volume `27` its type id (`cell->type` in C++) will be changed to *1* . Because target volume of our simulation is `25` and we know that this volume subject to random fluctuations we should be able to turn quite a few of cells in our simulation into cells of type id *1*

Note

During the course of the single MonteCarlo step a given cell may change its volume many times

We will only trigger cell type change when volume 27 or higher is reached when the cell increases its volume and therefore our code looks as follows:

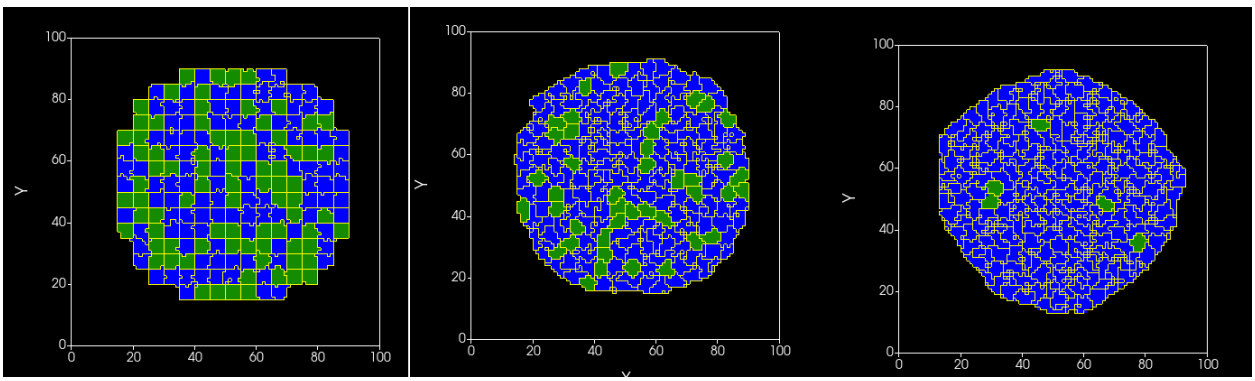
```
void SimpleVolumeTrackerPlugin::field3DChange(const Point3D &pt, CellG *newCell, CellG␣
↪*oldCell)

{

    // note: we only care about cells that reach volume 27 when they grow
    if (newCell) {
        if (newCell->volume >= 27) {
            newCell->type = 1;
        }
    }

}
```

After we compile it and run it we will see that relatively quickly most of the cells in the simulation will turn to cell type *1* (blue color)



This tiny code change concludes our next example.

10.1 Order in which plugins are called

In general order in which plugins are called depends on the order in which they are listed in the XML. However, certain plugins might require other plugins and in this case this order my get reshuffled. We will come back to this issue later.

One thing you should remember here though is, that changing cell type in a plugin might not be very safe because, what if after our `SimpleVolumeTracker` there is another plugin that actually relies on the type information and before it had a chance to be called our plugin messed up cell type configuration for given instance of the simulation? Fortunately, in our case we did not have such an issue, but it is a good idea to be aware of such situations and in general adjustments of cell parameters such as cell type, `targetVolume`, `lambdaVolumes` are best handled in the Steppables. In subsequent chapters we will show you how to build Steppables in C++.

CHAPTER

ELEVEN

SETTING UP WINDOWS COMPUTER FOR DEVELOPERZONE COMPILATION AND DEVELOPING NEW CC3D PLUGINS AND STEPPABLES IN C++

If you want tot develop plugins and steppables under windows you will need to install free Visual Studio 2015 Community Version. The installation of this package is straightforward but you need to make sure that you are installing C/C++ compilers when the installer gives you options to select which programming languages you would like to have support for. The best way to download Visual Studio is to get it directly from Microsoft website. Current link to visual studio download page is here: https://visualstudio.microsoft.com/vs/older-downloads/ . Just make sure you scroll down and find Visual Studio 2015. It has to be exactly this version. CompuCell3D compilation will likely not work with other versions. Once you download and install Visual Studio 2015 you are ready to start compiling Developer Zone projects and develop your own CompuCell3D plugins and steppables in C++.

CHAPTER

TWELVE

SETTING UP LINUX COMPUTER FOR DEVELOPERZONE COMPILATION AND DEVELOPING NEW CC3D PLUGINS AND STEPPABLES IN C++

If you are using linux computer , most likely you do not need to do any compiler setup. CC3D on Linux comes prepackaged with all compilers and it does not matter if you installed CC3D using automated installer or installed directly using `conda install` command.

CHAPTER

THIRTEEN

SETTING UP YOUR MAC FOR DEVELOPERZONE COMPILATION AND DEVELOPING NEW CC3D PLUGINS AND STEPPABLES IN C++

Starting with CC3D 4.3.0 when you install CC3D it will come with most of the tools needed to compile C+++ plugins and steppables. The only thing that you need in addition to this is to install `xcode-select` package To install this from the terminal run the following:

```
xcode-select --install
```

This is it and you should be ready to compile custom plugins and steppables written in C++

CHAPTER

FOURTEEN

SETTING UP YOUR MAC FOR CC3D COMPILATION VIA CONDA

Sometimes you may want to compile entire CC3D C++ code using conda build system. In general when compiling code via conda-build system you do not need to install anything - besides manking sure that your conda-build system works properly. To ensure that conda build system works properly from your `base` conda environment (it is important that this is `base` environment or else things may not work properly) run

```
conda install conda-build
```

This will install all utilities you need to build CC3D. Tools like swig, cmake, compilers etc will be downloaded and installed automatically just in time for compilation. We will only mention that Current version of CC3D uses clang compilers version 12. On Linux we use gcc compilers and on Windwos Visual Studio 2015 Community Version (free)

To compile CC3D on your Mac using conda-build system follow this procedure:

1. Install `xcode-select` - see above
2. install miniconda3 with Python 3.7 - https://repo.anaconda.com/miniconda/Miniconda3-py37_4.11.0-MacOSX-x86_64.sh .

Once you install miniconda in the `base` environment of newly installed miniconda install `conda-build` package

```
conda install conda-build
```

3. Get MacOS SDK 10.10 - https://github.com/phracker/MacOSX-SDKs or directly from https://github.com/phracker/MacOSX-SDKs/releases. Here is direct link to the actual compressed folder: https://github.com/phracker/MacOSX-SDKs/releases/download/11.3/MacOSX10.10.sdk.tar.xz Once you unpack move the content to `/opt` folder of your Mac. You need to be `admin` to do this. You should be able to see the following folder `/opt/MacOSX10.10.sdk` after the copy is complete

4. Clone CC3D repository

```
git clone https://github.com/CompuCell3D/CompuCell3D.git
```

5. Go to CC3D repository's `conda-recipes` folder:

```
cd <CC3D repository dir>/conda=recipe
```

6. Start compilation by typing

```
conda build . -c conda-forge -c compucell3d
```

After a while you should have CC3D conda package ready

CHAPTER

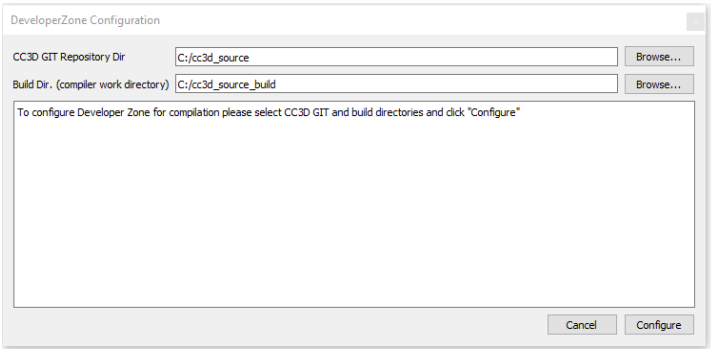
FIFTEEN

CONFIGURING DEVELOPERZONE PROJECTS FOR COMPILATION

From technical viewpoint `DeveloperZone` is a folder that contains source code for additional plugins and steppables written in C++. Depending on your needs, sometimes, you want to write high-performance CC3D module that runs much faster than equivalent Python code. Up until version 4.3.0 of CC3D developing C++ modules was a little bit involved because it required users to install and configure appropriate compilers that will work with provided binaries, performing CMake configuration - the challenge here was to make sure that all Cmake variables point to appropriate directories, that Python version identified by Cmake matches the one with which CC#D was compiled etc… In practice this process was often perceived as quite error-prone.

Starting with version 4.3.0 of CC3D we provide one-click configurator for "DeveloperZone" All that is required from the user is one time setup of compiler (on Windows you will install Visual Studio 2015 Community Edition, and on Mac you need to install xcode-select package - all described in sections above. On linux you will likely not need any additional setup).

Once you set up compilers (and install binaries for CC3D) open Twedit++ and go to `CC3D C++ -> DeveloperZone ...` . This will open the following dialog:



Before going any further, make sure you you have a working copy of the CC3D source code. The best way is to clone CC3D source code repository. If you have git installed on your system you are ready to go. If not you can easily do it by running `conda-shell` script from CC3D installation folder. Assuming your CC3D is installed into `c:\CompuCell3D` (on Windows) you would run the following:

```
cd c:\
c:\CompuCell3D\conda-shell.bat
```

then :

```
conda install -c conda-forge git
```

At this point you should have `git` installed within base environment of the miniconda distribution that is bundled with CC3D. In general to make use of any conda tools you would first need to run `conda-shell` each time you open new terminal.

Let's clone CC3D source code now. In the terminal where you previously ran `conda-shell.bat`, do the following

```
cd c:\cc3d_source
git clone https://github.com/CompuCell3D/CompuCell3D.git .
```

This will clone (download) CC3D source code and place it in `c:\cc3d_source`

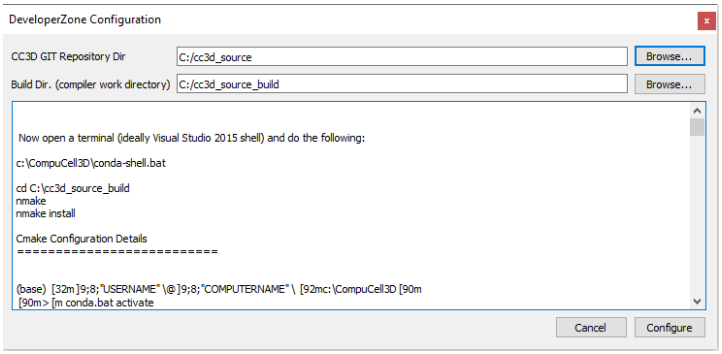
Now let's make build directory. This is a directory where compilers will place temporary compilation objects:

```
cd c:\
mkdir cc3d_source_build
```

Warning

It is important to create a fresh (empty) build directory before you can configure DeveloperZone configuration. CC3D cannot use build directory that is non empty

Now, fill in full path to CC3D repository (`c:\cc3d_source`) and to build folder (`c:\cc3d_source_build`) and click `Configure` button in the bottom right corner of the dialog. Configuration process will start. After it is done the dialog should display summary of what to do next:



On Windows, we are asked to open a terminal (ideally Visual Studio 2015 64bit shell - search for VS2015 x64 native tools in main search menu of Windows operating system, or simply open any terminal on windows) and run the

```
c:\CompuCell3D\conda-shell.ba
```

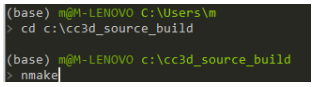
This, in addition to activating base miniconda environment will "preconfigure" the terminal for compilation using Visual Studio 2015 Tools. You only need to run this `conda=shell.bat` command for "regular" terminal. If you opened Visual Studio Terminal you may skip this step

Then you run the following:

```
cd C:\cc3d_source_build

nmake
nmake install
```

First command changes directory to the directory that we designated for storing temporary compilation files. This is where the Makefile were generated to. Next, we run windows version of `make` called `nmake`.



Once compilation finishes

```
c:\cc3d_source\compucell3d\core\compucell3d\PluginManager.h(108): warning C4251: 'CompuCell3D::PluginManager<CompuCell3D::Step
pable>::libExtension': class 'std::basic_string<char,std::char_traits<char>,std::allocator<char>>' needs to have dll-interface
 to be used by clients of class 'CompuCell3D::PluginManager<CompuCell3D::Steppable>'
c:\cc3d_source\compucell3d\core\compucell3d\field3d\Field3DImpl.h(70): warning C4018: '<': signed/unsigned mismatch
c:\cc3d_source\compucell3d\core\compucell3d\field3d\Field3DImpl.h(58): note: while compiling class template member function 'C
ompuCell3D::Field3DImpl<float>::Field3DImpl(const CompuCell3D::Dim3D,const T &)'
        with
        [
            T=float
        ]
C:\cc3d_source\CompuCell3D\core\CompuCell3D/Field3D/Array3D.h(133): note: see reference to function template instantiation 'Co
mpuCell3D::Field3DImpl<float>::Field3DImpl(const CompuCell3D::Dim3D,const T &)' being compiled
        with
        [
            T=float
        ]
C:\cc3d_source\CompuCell3D\core\CompuCell3D/Field3D/Array3D.h(129): note: see reference to class template instantiation 'Compu
Cell3D::Field3DImpl<float>' being compiled
[100%] Linking CXX shared module _CompuCellExtraModules.pyd
CompuCellExtraModulesPYTHON_wrap.cxx.obj : MSIL .netmodule or module compiled with /GL found; restarting link with /LTCG; add
/LTCG to the link command line to improve linker performance
LINK : warning LNK4075: ignoring '/INCREMENTAL' due to '/LTCG' specification
   Creating library CompuCellExtraModules.lib and object CompuCellExtraModules.exp
Generating code
Finished generating code
CompuCellExtraModulesPYTHON_wrap.cxx.obj : MSIL .netmodule or module compiled with /GL found; restarting link with /LTCG; add
/LTCG to the link command line to improve linker performance
LINK : warning LNK4075: ignoring '/INCREMENTAL' due to '/LTCG' specification
   Creating library CompuCellExtraModules.lib and object CompuCellExtraModules.exp
Generating code
Finished generating code
[100%] Built target CompuCellExtraModules

(base) m@M-LENOVO c:\cc3d_source_build
>
```

we install the compiled modules.

```
Finished generating code
[100%] Built target CompuCellExtraModules

(base) m@M-LENOVO c:\cc3d_source_build
> nmake install

Microsoft (R) Program Maintenance Utility Version 14.00.23026.0
Copyright (C) Microsoft Corporation.  All rights reserved.

[ 16%] Built target CustomCellAttributeSteppableShared
[ 33%] Built target HeterotypicBoundaryLengthShared
[ 50%] Built target GrowthSteppableShared
[ 66%] Built target SimpleVolumeShared
[ 83%] Built target VolumeMeanShared
[ 88%] Built target CompuCellExtraModules_swig_compilation
[100%] Built target CompuCellExtraModules
Install the project...
-- Install configuration: "RelWithDebInfo"
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DCustomCellAttributeSteppable.l

-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DCustomCellAttributeSteppable.d

-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DHeterotypicBoundaryLength.lib
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DHeterotypicBoundaryLength.dll
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DGrowthSteppable.lib
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DGrowthSteppable.dll
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DPlugins/CC3DSimpleVolume.lib
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DPlugins/CC3DSimpleVolume.dll
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DVolumeMean.lib
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCell3DSteppables/CC3DVolumeMean.dll
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/_CompuCellExtraModules.pyd
-- Installing: c:/CompuCell3D/Miniconda3/Lib/site-packages/cc3d/cpp/CompuCellExtraModules.py

(base) m@M-LENOVO c:\cc3d_source_build
>
```

If you look carefully at the output screen you will see that the modules we compiled will get installed into subfolders of `c:\CompuCell3D\Miniconda3` which is Miniconda distribution that is part of CC3D installation. This is exactly what we want. In other words, with one click and few simple command line commands we were able to compile a set of demo extensions modules written in C++. This is significant because this simple procedure allows you to easily add new C++ modules and significantly speedup your simulation. From now on you can focus on coding rather than figuring out of how to set up compilation

CHAPTER

SIXTEEN

BUILDING STEPPABLE

It is probably best to start discussing extension of CC3D by showing a relatively simple example of a steppable written in C++. In typical scenario steppables are written in Python. There are three main reasons for that **1)** No compilation is required. **2)** The code is more compact and easier to write than C++. **3)** Python has a rich set of libraries that make scientific computation easily accessible. However, writing a steppable in C++ is not that much more difficult, as you will see shortly, and you are almost guaranteed that your code will run orders of magnitude faster. Let me rephrase this last sentence - a **typical** code written in C++ is orders of magnitude faster than equivalent code written in pure Python. Since most of the steppable code consists of iterating over all cells and adjusting their attributes, C++ will perform this task much faster.

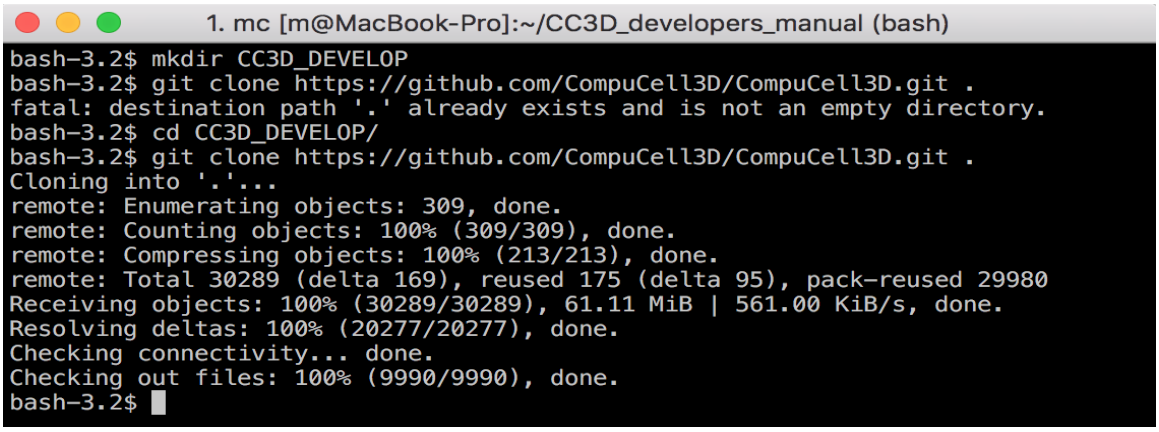
16.1 Getting started

Before you start developing CC3D C++ extension modules, you need to clone CC3D repository.

```
mkdir CC3D_DEVELOP
cd CC3D_DEVELOP
git clone https://github.com/CompuCell3D/CompuCell3D.git .
```

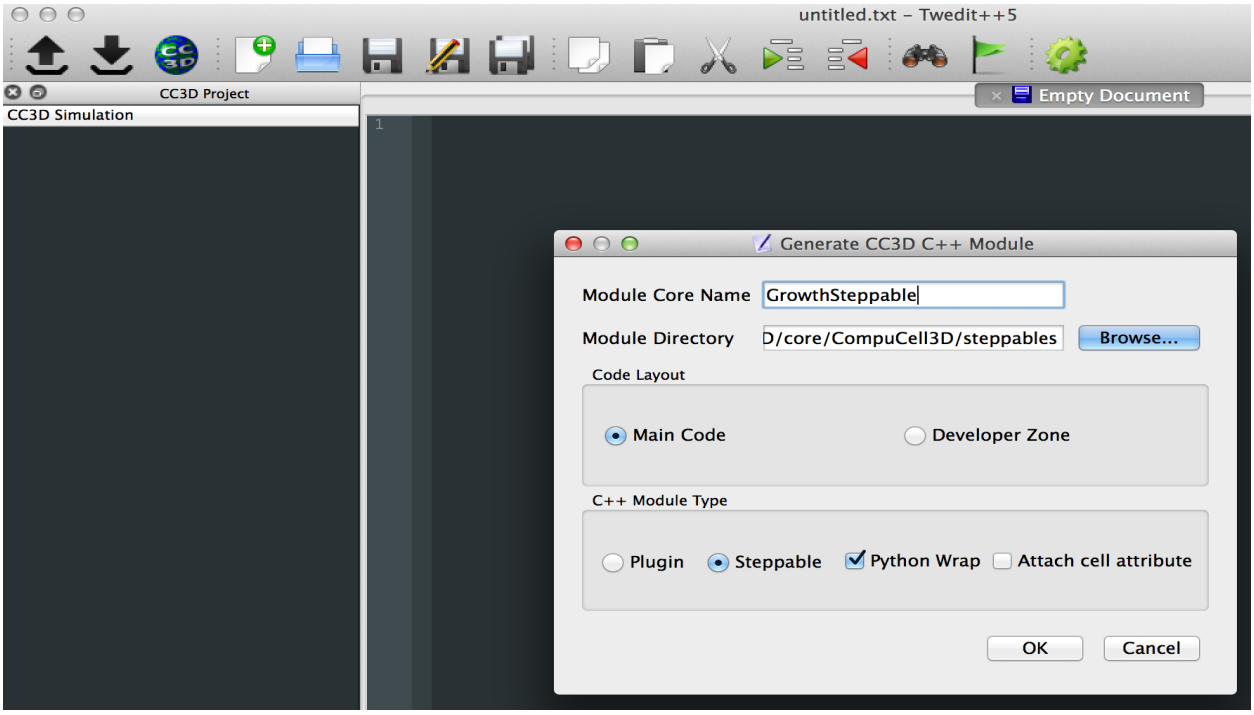
It is optional to checkout a particular branch of CC3D, but most often you will work with `master` branch. If , however, you want to checkout a branch - you would type something like this:

```
git checkout 4.0.0
```



At this point you have complete code in `CC3D_DEVELOP` directory.

Now we open Twedit++ - you need to have "standard" installation of CC3D on your machine available - and go to `CC3D C++` menu and choose `Generate New Module...` entry and fill out the dialog box:



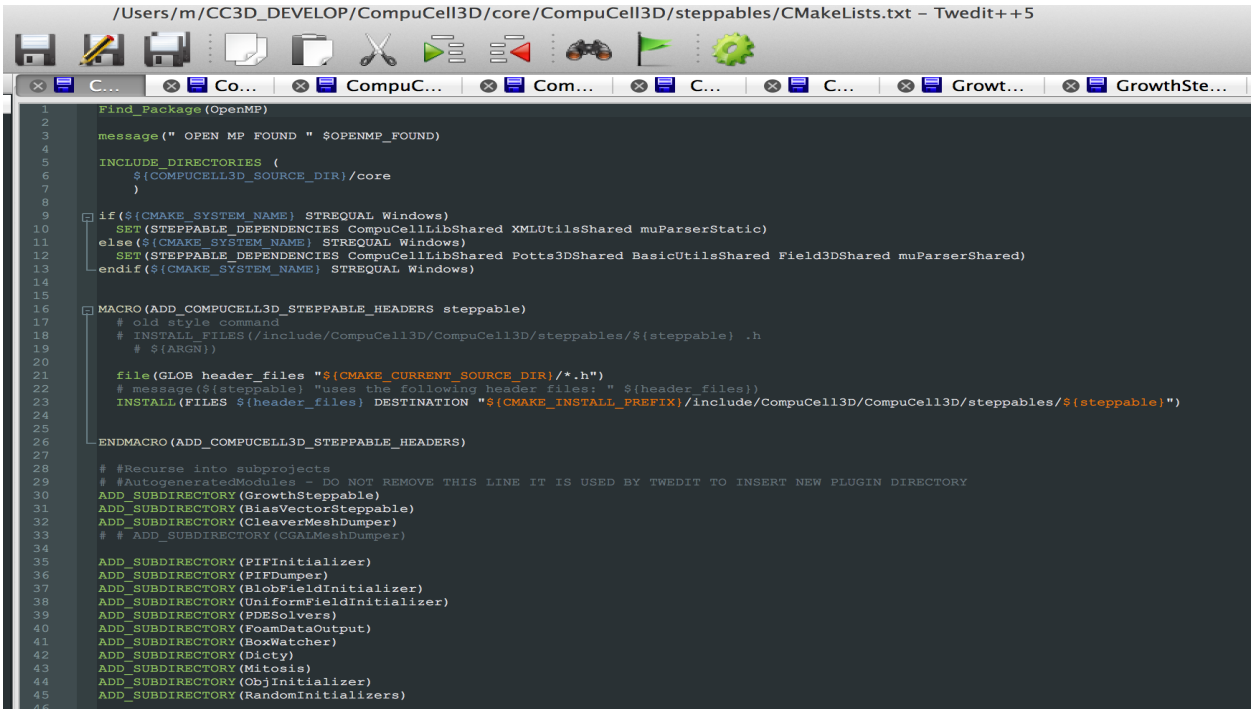
Note

In this example we show how to generate steppable code template in the "main" CC3D code. However, a more frequently used scenario is to Generate steppable code in "DeveloperZone" folder. We will show it in the subsequent chapter

This is exactly what we did:

1. We specify a name of a steppable as `GrowthSteppable`
2. We specify the location of when steppable code is stored `/Users/m/CC3D_DEVELOP/CompuCell3D/core/CompuCell3D/steppables`. Note, that we point to the cloned CC3D repository that we originally stored in `CC3D_DEVELOP` subdirectory. It happens that the path to this repository is `/Users/m/CC3D_DEVELOP`.
3. We select **Steppable** radio in the **C++ Module Type** panel. We also check `Python Wrap` checkbox to allow generation of Python bindings of this steppable.

When we press `OK` button Twedit++ will generate a complete set of template files that could be compiled as-is and the steppable will run. Obviously our goal is to modify template file to generate steppable w want. In current implementation of CC3D Twedit++ generates or modifies approximately 10 files.



As you can see in the `CMakeLists.txt` file Twedit++ modified this file and added line `ADD_SUBDIRECTORY(GrowthSteppable)`

Now, let us focus on modifying template files and creating a steppable (`GrowthSteppable`) we specify growth rate in the XMl and allow modification of this rate from Python.

Let's first examine the header of the `GrowthSteppable` class:

```
#ifndef GROWTHSTEPPABLESTEPPABLE_H
#define GROWTHSTEPPABLESTEPPABLE_H



#include <CompuCell3D/CC3D.h>
#include "GrowthSteppableDLLSpecifier.h"


namespace CompuCell3D {

  template <class T> class Field3D;

  template <class T> class WatchableField3D;


    class Potts3D;
    class Automaton;
    class BoundaryStrategy;
    class CellInventory;
    class CellG;

  class GROWTHSTEPPABLE_EXPORT GrowthSteppable : public Steppable {
```

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```
    WatchableField3D<CellG *> *cellFieldG;
    Simulator * sim;
    Potts3D *potts;
    CC3DXMLElement *xmlData;
    Automaton *automaton;
    BoundaryStrategy *boundaryStrategy;
    CellInventory * cellInventoryPtr;


    Dim3D fieldDim;
  public:
    GrowthSteppable ();
    virtual ~GrowthSteppable ();
    // SimObject interface
    virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);
    virtual void extraInit(Simulator *simulator);
    //steppable interface
    virtual void start();
    virtual void step(const unsigned int currentStep);
    virtual void finish() {}
    //SteerableObject interface
    virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false);
    virtual std::string steerableName();
     virtual std::string toString();
  };
};
#endif
```

Each steppable defines `virtual void start()`, `virtual void step(const unsigned int currentStep)` and `virtual void finish()` functions. They have exactly the same role as analogous functions in Python scripting. The oly differentce is that C++ steppables will be called **before** Python steppables

Let us check the generated implementation file of the Steppable (the `.cpp` file):

```
#include <CompuCell3D/CC3D.h>
using namespace CompuCell3D;
using namespace std;
#include "GrowthSteppable.h"
GrowthSteppable::GrowthSteppable() : cellFieldG(0),sim(0),potts(0),xmlData(0),
↪boundaryStrategy(0),automaton(0),cellInventoryPtr(0){}

GrowthSteppable::~GrowthSteppable() {

}

void GrowthSteppable::init(Simulator *simulator, CC3DXMLElement *_xmlData) {

  xmlData=_xmlData;

  potts = simulator->getPotts();

  cellInventoryPtr=& potts->getCellInventory();

  sim=simulator;

  cellFieldG = (WatchableField3D<CellG *> *)potts->getCellFieldG();

  fieldDim=cellFieldG->getDim();

  simulator->registerSteerableObject(this);

  update(_xmlData,true);


}

void GrowthSteppable::extraInit(Simulator *simulator){

    //PUT YOUR CODE HERE
}

void GrowthSteppable::start(){

  //PUT YOUR CODE HERE

}

void GrowthSteppable::step(const unsigned int currentStep){

    //REPLACE SAMPLE CODE BELOW WITH YOUR OWN

    CellInventory::cellInventoryIterator cInvItr;
```

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```
    CellG * cell=0;

    cerr<<"currentStep="<<currentStep<<endl;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )

    {

        cell=cellInventoryPtr->getCell(cInvItr);

        cerr<<"cell.id="<<cell->id<<" vol="<<cell->volume<<endl;

    }

}

void GrowthSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    //PARSE XML IN THIS FUNCTION

    //For more information on XML parser function please see CC3D code or lookup XML␣
↪utils API

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

   set<unsigned char> cellTypesSet;

    CC3DXMLElement * exampleXMLElem=_xmlData->getFirstElement("Example");

    if (exampleXMLElem){

        double param=exampleXMLElem->getDouble();

        cerr<<"param="<<param<<endl;

        if(exampleXMLElem->findAttribute("Type")){

            std::string attrib=exampleXMLElem->getAttribute("Type");

            // double attrib=exampleXMLElem->getAttributeAsDouble("Type"); //in case␣
↪attribute is of type double

            cerr<<"attrib="<<attrib<<endl;

        }

    }
```

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```
    //boundaryStrategy has information about pixel neighbors

    boundaryStrategy=BoundaryStrategy::getInstance();

}

std::string GrowthSteppable::toString(){

   return "GrowthSteppable";

}

std::string GrowthSteppable::steerableName(){

   return toString();

}
```

The step and start``functions are the first function we will modify. In its current implementation the generated ``step function already contains helpful code but start function will be rewritten. Let's take a look:

```
void GrowthSteppable::start(){


}

    void GrowthSteppable::step(const unsigned int currentStep){

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

    cerr<<"currentStep="<<currentStep<<endl;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )

    {

        cell = cellInventoryPtr->getCell(cInvItr);

        cerr << "cell.id=" << cell->id << " vol=" << cell->volume << endl;

    }

}
```

The `for` loop iterates over inventory of cells and prints cell id and cell volume. To iterate over cell inventory we are using `cellInventoryPtr` which is a pointer to `CellInventory` object. The class for this object (`CellInventory`) is defined in `Potts3D/CellInventory.h` and implementation is in `Potts3D/CellInventory.cpp`. Internally, we are using STL(Standard Template Library - C++) maps to keep track of cells. The statement

cellInventoryPtr->cellInventoryBegin() returns an iterator to cell inventory. If you look closely at the implementation files the container we are using as a cell inventory is std::map<CellIdentifier,CellG *> and CellIdentifier contains cell id and cluster id to uniquely identify cells. Therefore iteration over cell inventory is simply iteration over STL map. If you are not familiar with concept of iterators and containers of STL we recommend that you look up basic C++ tutorials for example: https://www.tutorialspoint.com/cplusplus/cpp_stl_tutorial .

Let us now modify the above start and step functions and implement first version of growth steppable:

```
void GrowthSteppable::start(){

    CellInventory::cellInventoryIterator cInvItr;
    CellG * cell = 0;

    for (cInvItr = cellInventoryPtr->cellInventoryBegin(); cInvItr != cellInventoryPtr->
↪cellInventoryEnd(); ++cInvItr)
    {

        cell = cellInventoryPtr->getCell(cInvItr);
        cell->targetVolume = 25.0;
        cell->lambdaVolume = 2.0;
    }

}

    void GrowthSteppable::step(const unsigned int currentStep){

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

    float growthRate = 1.0;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )

    {

        cell = cellInventoryPtr->getCell(cInvItr);
        cell->targetVolume += growthRate ;

    }

}
```

When we create cells they all have targetVolume and lambdaVolume set to 0.0 and thus volume constraint does nothing. We fix it by setting those parameters for each cell in the start function.

If you are familiar with CC3D Python scripting you will quickly find analogies. The only thing we added was the following statement cell->targetVolume += growthRate ;

When we compile and run this example the cells' target volume will increase by amount hardcoded in the growthRate variable which in our case is 1.0.

Let's take it to the next level (slowly). Now we will write a code that increases target volume of cells but only for the first 100 MCS and only if cell type is equal to 1.

```
    void GrowthSteppable::step(const unsigned int currentStep){

    if (currentStep > 100)
        return;

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

    float growthRate = 1.0;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )

    {

        cell = cellInventoryPtr->getCell(cInvItr);
        if (cell->type == 1){
            cell->targetVolume += growthRate ;
        }

    }

}
```

First thing we do in this steppable is checking if current MCS is greater than `100` and if so we return. Inside the loop we added `if (cell->type == 1)` check that allows increase of target volume only if cell is of type `1`. Small digression here. If you want to print cell type to the screen you need to use the following syntax:

```
cerr << "cell type=" << (int)cell->type <<endl;
```

As you can see we are performing type cast to `int`. This is because cell type (defined in `Potts3D/Cell.h`) is defined as `unsigned char`. Consequently CC3D allows only 256 cell types, which at first sight might look limiting but in practice is more than enough.

In the previous examples we hard-coded the value of growth rate using `float growthRate = 1.0;`. This is not an optimal solution. What if you want to run 5 simulations simultaneously each one with different value of growth rate. If you hard-code values you would need to have 5 distinct compilations of CC3D available. Clearly, hard-coding is not scalable. We need better solution. It is time to learn how to parse XML in C++ code

16.2 Parsing XML in C++

Building flexible code requires that we provide some sensible configuration mechanism via which users can customize their simulation without the need to recompile code. In CC3D we have two ways of achieving it **1)** XML **2)** Python scripting. It is up to you which one you use and we will teach you how to use both approaches. For now let's start with XML parsing.

All C++ CC3D Plugins and Steppables define virtual function `update(CC3DXMLElement *_xmlData, bool _fullInitFlag)`. This function takes two arguments: pointer to XML element `_xmlData` (that CC3D initializes to be the root element of the particular Plugin or Steppable) and a flag `_fullInitFlag` that specifies if full initialization of the module is required or not.

Suppose that our XML will look as follows:

```
<Steppable Type="GrowthSteppable">
    <GrowthRate>1.0</GrowthRate>
</Steppable>
```

We would parse this XML in C++ using the following code:

```
void GrowthSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

   set<unsigned char> cellTypesSet;

    CC3DXMLElement * growthElem = _xmlData->getFirstElement("GrowthRate");

    if (growthElem){

        this->growthRate = growthElem->getDouble();

    }

    //boundaryStrategy has information about pixel neighbors

    boundaryStrategy=BoundaryStrategy::getInstance();

}
```

As we mentioned before `_xmlData` points to `<Steppable Type="GrowthSteppable">`. We need to get the child of this element *i.e.* `<GrowthRate>1.0</GrowthRate>`. Since we know that there is only one child element (let's say we make such constraint for now - we will relax it later) we use the following code:

```
CC3DXMLElement * growthElem = _xmlData->getFirstElement("GrowthRate");
```

The `getFirstElement` method returns a pointer to a child element that is of the form

```
<GrowthRate ...>...</GrowthRate>
```

The returned pointer can be `NULL` if suitable child element cannot be found. This is why we add `if (growthElem)` check. Assuming that the `<GrowthRate>` child exist we read its `cdata` part. For any XML element , cdata part (cdata stands for character data) is the part that sits between closing > and opening < brackets of XML element. For example in

```
<GrowthRate>1.0</GrowthRate>
```

the `cdata` part is 1.0. The `CC3DXMLElement` has several methods that read and convert cdata to appropriate C++ type. Here we are using `getDouble()`

```
this->growthRate = growthElem->getDouble();
```

Obviously, `CC3DXMLElement` defines more methods to convert character data to required type (`getInt`, `getBool` , *etc.*. . .) They are defined in `XMLUtils/CC3DXMLElement.h`

In order for this code to work we need to define growthRate inside `GrowthSteppable` class header - we can do it as follows:

```
class GROWTHSTEPPABLE_EXPORT GrowthSteppable : public Steppable {

  WatchableField3D<CellG *> *cellFieldG;

  Simulator * sim;

  Potts3D *potts;

  CC3DXMLElement *xmlData;

  Automaton *automaton;

  BoundaryStrategy *boundaryStrategy;

  CellInventory * cellInventoryPtr;

  Dim3D fieldDim;

public:

  GrowthSteppable ();

  virtual ~GrowthSteppable ();

  double growthRate;

  ...
  }
```

With those changes we can rewrite our `step` function as:

```
void GrowthSteppable::step(const unsigned int currentStep){

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

   if (currentStep > 100)
       return;


    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )
    {

        cell=cellInventoryPtr->getCell(cInvItr);

        if (cell->type == 1){
            cell->targetVolume += this->growthRate;
        }
```

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```
    }

}
```

It is almost the same implementation as before except we use `cell->targetVolume += this->growthRate;` instead of `cell->targetVolume += growthRate;`

The `this->growthRate` gets initialized based on the input provided in

```
<Steppable Type="GrowthSteppable">
    <GrowthRate>1.0</GrowthRate>
</Steppable>
```

If we change it to

```
<Steppable Type="GrowthSteppable">
    <GrowthRate>2.0</GrowthRate>
</Steppable>
```

and rerun the simulation the rate of increase of target volume will be 2.0. All the changes we make to the growth rate now do not require recompilation but only chenges int he XML file, exactly how CC3D is designed to work. Next we will learn how to parse attributes of the XML elements. As a motivating example we will specify different growth rates for different cell types.

16.2.1 Parsing XMl Attributes

If we want our simulation to have different growth rates for different cell types we need to store them in *e.g.* STL map and we need to modify header of the `GrowthSteppable` to look as follows:

```
class GROWTHSTEPPABLE_EXPORT GrowthSteppable : public Steppable {

  WatchableField3D<CellG *> *cellFieldG;

  Simulator * sim;

  Potts3D *potts;

  CC3DXMLElement *xmlData;

  Automaton *automaton;

  BoundaryStrategy *boundaryStrategy;

  CellInventory * cellInventoryPtr;

  Dim3D fieldDim;

public:

  GrowthSteppable ();

  virtual ~GrowthSteppable ();
```

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```
  std::map<unsigned int, double> growthRateMap;

  ...
  }
```

We replaced `double growthRate` with `std::map<unsigned int, double> growthRateMap;` The key of the map is cell type and the value is growth rate. Now we need to design and parse XML that will allow users to specify required data. Let us try the following syntax:

```
<Steppable Type="GrowthSteppable">
    <GrowthRate CellType="1">1.3</GrowthRate>
    <GrowthRate CellType="2">1.7</GrowthRate>
</Steppable>
```

I case you wonder what I mean by "trying out syntax" it means that it is up to you to design XML syntax in such a way that it allows you to specify model in the way you want. The above example fulfills this requirement because we specify different growth rates for different cell types. However, we could also come up with a different way of specifying the same information:

```
<Steppable Type="GrowthSteppable">
    <GrowthRate CellType="1" Rate="1.3"/>
    <GrowthRate CellType="2" Rate="1.7"/>
</Steppable>
```

Both approaches are OK.

Let us write the `update` function that will parse first of the above XMLs:

```
void GrowthSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

    set<unsigned char> cellTypesSet;

    CC3DXMLElementList growthVec = _xmlData->getElements("GrowthRate");

    for (int i = 0; i < growthVec.size(); ++i) {
        unsigned int cellType = growthVec[i]->getAttributeAsUInt("CellType");
        double growthRateTmp = growthVec[i]->getDouble();
        this->growthRateMap[cellType] = growthRateTmp;
    }


    //boundaryStrategy has information about pixel neighbors
    boundaryStrategy=BoundaryStrategy::getInstance();

}
```

The code is slightly different this time because we expect multiple entries of the type `<GrowthRate CellType="xxx" Rate="yyy"/>`. Therefore, by writing the code:

```
CC3DXMLElementList growthVec = _xmlData->getElements("Rate");
```

we ensure that CC3D will return a list (actually it is implemented as an STL vector) of XML element pointers that start with `<GrowthRate ...>` . Next, we iterate over the vector of XML element pointers and notice that `growthVec[i]` returns a pointer to XML element pointer and we query this element. First, we read and convert to `unsigned int` value of `CellType` attribute:

```
unsigned int cellType = growthVec[i]->getAttributeAsUInt("CellType");
```

The next line:

```
double growthRateTmp = growthVec[i]->getDouble();
```

should be familiar already because it reads the value of `cdata` of `<GrowthRate CellType="1">1.3</GrowthRate>`

Once we extracted cell type and actual growth rate from a single element we store those values in `this->growthRateMap` map:

```
this->growthRateMap[cellType] = growthRateTmp;
```

Note

We are not performing any error checks in the above code and assume that users enter reasonable values. In the production code we would monitor for possible errors but this extra code would make this introductory manual a bit too confusing

If we wanted to parse second syntax where we specify growth rate as and attribute rather than `cdata` :

```
<Steppable Type="GrowthSteppable">
    <GrowthRate CellType="1" Rate="1.3"/>
    <GrowthRate CellType="2" Rate="1.7"/>
</Steppable>
```

we would need to make only small modification:

```
void GrowthSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

    set<unsigned char> cellTypesSet;

    CC3DXMLElementList growthVec = _xmlData->getElements("GrowthRate");

    for (int i = 0; i < growthVec.size(); ++i) {
        unsigned int cellType = growthVec[i]->getAttributeAsUInt("CellType");
        double growthRateTmp = growthVec[i]->getAttributeAsDouble("GrowthRate");
        this->growthRateMap[cellType] = growthRateTmp;
    }
```

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```
    //boundaryStrategy has information about pixel neighbors
    boundaryStrategy=BoundaryStrategy::getInstance();

}
```

The code differs from previous parsing code by only one line:

```
double growthRateTmp = growthVec[i]->getAttributeAsDouble("GrowthRate");
```

As usual for a complete list of functions that read and convert XML attributes to concrete C++ types , check `XMLUtils/CC3DXMLElement.h`

In order to take advantage of the specification of growth rate on a per-cell-type basis we modify step function as follows:

```
void GrowthSteppable::step(const unsigned int currentStep){

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

   if (currentStep > 100)
      return;

    std::map<unsigned int, double>::iterator mitr;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )
    {

        cell=cellInventoryPtr->getCell(cInvItr);

        mitr = this->growthRateMap.find((unsigned int)cell->type);

        if (mitr != this->growthRateMap.end()){
            cell->targetVolume += mitr->second;
        }

    }

}
```

We declare an iterator to the `std::map<unsigned int, double>`. HInt: iterator is like a pointer and in the case of map iterator will have two components `mitr->first` which will be a key of `this->growthRateMap` map (in our case a key is a cell type) and `mitr->second` which will point to a value of the `this->growthRateMap` which in our case is a growth rate.

When we get a new cell first thing we do is to check if iterator pointing to a pair of (cell type, growth rate) exist:

```
mitr = this->growthRateMap.find((unsigned int)cell->type);
```

If such entry exists in the `this->growthRateMap` then this iterator will point to a value different than `this->growthRateMap.end()` and in such a case we know that `mitr->second` points to a growth rate for a cell type given by `cell->type`. We simply increase target volume of such cell by the growth rate. This logic is code up in the following if statement":

```
if (mitr != this->growthRateMap.end()){
    cell->targetVolume += mitr->second;
}
```

The presented example went over a theory of how to build a basic steppable and integrate it with main CC3D code. In the next tutorial we will present the same steppable but we will build it in the `DevelopeZone` folder of CC3D. The idea here is that this new steppable can live outside main CC3D code and still be accessible by the installed binaries.

CHAPTER

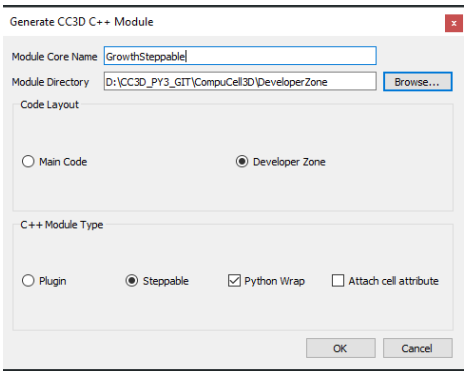
SEVENTEEN

BUILDING GROWTH STEPPABLE IN THE DEVELOPER ZONE FOLDER

Quite often you will want to build a steppable in a "non-intrusive" way *i.e.* without adding it to the main CC3D code-base. The way to do it is to utilize functionality of `DeveloperZone`.

This time we will use Windows system and our CC3D git repository is cloned to `D:\CC3D_PY3_GIT\CompuCell3D`

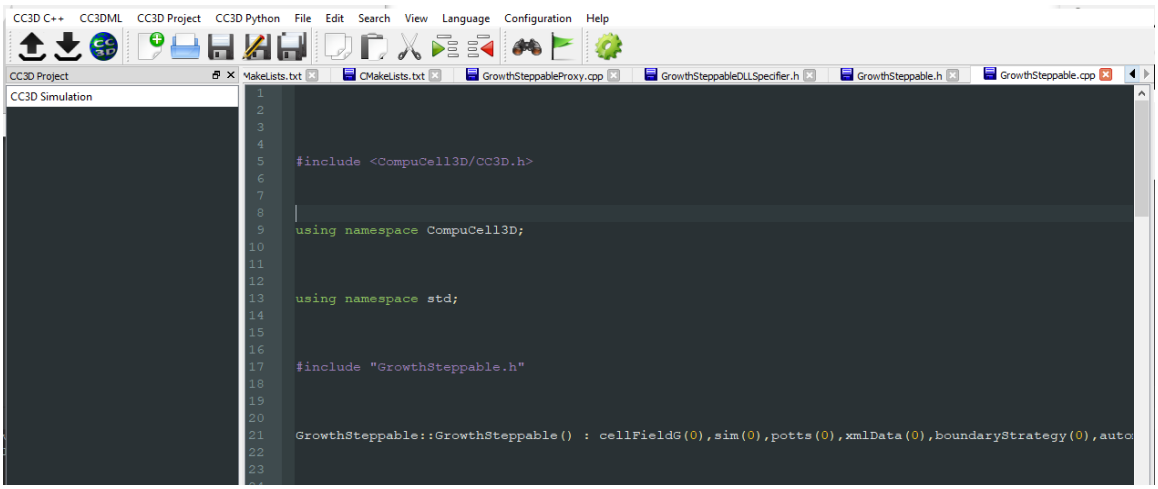
To add a steppable or plugin in the DeveloperZone you open up Twedit and from `CC3D C++` menu select `Generate New Module...`.



Notice that in the `Module Directory` in the dialog box we put `D:\CC3D_PY3_GIT\CompuCell3D\DeveloperZone`. Previously we put there a path to the Steppable folder in the main CC3D Code base (give where our repository is cloned this path would be `D:\CC3D_PY3_GIT\CompuCell3D\core\CompuCell3D\steppables\`)

Notice that we also checked `Python Wrap` option to generate Python bindings. We will show you how you ca be creative here and leverage both XML and Python as a way to pass parameters to the Steppable. As you remember you do not have to generate Python bindings and it is perfectly OK to to stick with C++ and XML.

After we press `OK` button Twedit++ will generate , a template Steppable code:



Now we copy code from our earlier example into appropriate files - we are only showing files that we modified: `GrowthSteppable.h` :

```
#ifndef GROWTHSTEPPABLESTEPPABLE_H
#define GROWTHSTEPPABLESTEPPABLE_H
#include <CompuCell3D/CC3D.h>
#include "GrowthSteppableDLLSpecifier.h"

namespace CompuCell3D {

    template <class T> class Field3D;

    template <class T> class WatchableField3D;

    class Potts3D;

    class Automaton;

    class BoundaryStrategy;

    class CellInventory;

    class CellG;

  class GROWTHSTEPPABLE_EXPORT GrowthSteppable : public Steppable {

    WatchableField3D<CellG *> *cellFieldG;

    Simulator * sim;

    Potts3D *potts;

    CC3DXMLElement *xmlData;

    Automaton *automaton;

    BoundaryStrategy *boundaryStrategy;

```

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```
    CellInventory * cellInventoryPtr;

    Dim3D fieldDim;

  public:

    GrowthSteppable ();

    virtual ~GrowthSteppable ();

    std::map<unsigned int, double> growthRateMap;

    // SimObject interface

    virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);

    virtual void extraInit(Simulator *simulator);


    //steppable interface

    virtual void start();

    virtual void step(const unsigned int currentStep);

    virtual void finish() {}


    //SteerableObject interface

    virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false);

    virtual std::string steerableName();

    virtual std::string toString();

  };

};

#endif
```

and GrowthSteppable.cpp

```
#include <CompuCell3D/CC3D.h>
using namespace CompuCell3D;
using namespace std;
#include "GrowthSteppable.h"


GrowthSteppable::GrowthSteppable() :
cellFieldG(0),sim(0),potts(0),xmlData(0),
```

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```
boundaryStrategy(0),automaton(0),cellInventoryPtr(0){}

GrowthSteppable::~GrowthSteppable() {

}

void GrowthSteppable::init(Simulator *simulator, CC3DXMLElement *_xmlData) {

  xmlData=_xmlData;

  potts = simulator->getPotts();

  cellInventoryPtr=& potts->getCellInventory();

  sim=simulator;

  cellFieldG = (WatchableField3D<CellG *> *)potts->getCellFieldG();

  fieldDim=cellFieldG->getDim();

  simulator->registerSteerableObject(this);

  update(_xmlData,true);
}

void GrowthSteppable::extraInit(Simulator *simulator){

}

void GrowthSteppable::start(){

    CellInventory::cellInventoryIterator cInvItr;
    CellG * cell = 0;

    for (cInvItr = cellInventoryPtr->cellInventoryBegin(); cInvItr != cellInventoryPtr->
↪cellInventoryEnd(); ++cInvItr)
    {

        cell = cellInventoryPtr->getCell(cInvItr);
        cell->targetVolume = 25.0;
        cell->lambdaVolume = 2.0;
    }
}

void GrowthSteppable::step(const unsigned int currentStep){

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell=0;

   if (currentStep > 100)
       return;
```

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```
    std::map<unsigned int, double>::iterator mitr;

    for(cInvItr=cellInventoryPtr->cellInventoryBegin() ; cInvItr !=cellInventoryPtr->
↪cellInventoryEnd() ;++cInvItr )
    {

        cell=cellInventoryPtr->getCell(cInvItr);

        mitr = this->growthRateMap.find((unsigned int)cell->type);

        if (mitr != this->growthRateMap.end()){
            cell->targetVolume += mitr->second;
        }

    }

}

void GrowthSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

    set<unsigned char> cellTypesSet;

    CC3DXMLElementList growthVec = _xmlData->getElements("GrowthRate");

    for (int i = 0; i < growthVec.size(); ++i) {
        unsigned int cellType = growthVec[i]->getAttributeAsUInt("CellType");
        double growthRateTmp = growthVec[i]->getAttributeAsDouble("Rate");
        this->growthRateMap[cellType] = growthRateTmp;
    }

    //boundaryStrategy has information about pixel neighbors
    boundaryStrategy=BoundaryStrategy::getInstance();

}

std::string GrowthSteppable::toString(){

   return "GrowthSteppable";
}

std::string GrowthSteppable::steerableName(){

   return toString();
}
```

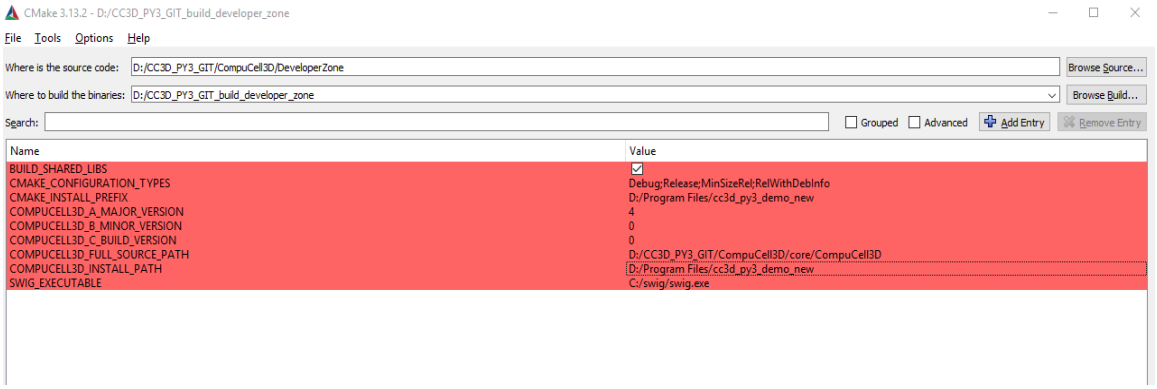
As you can see based on the previous discussion the `update` function where we parse XML is designed to handle the following syntax for the GrowthSteppable:

```
<Steppable Type="GrowthSteppable">
    <GrowthRate CellType="1" Rate="1.3"/>
    <GrowthRate CellType="2" Rate="1.7"/>
</Steppable>
```

Note

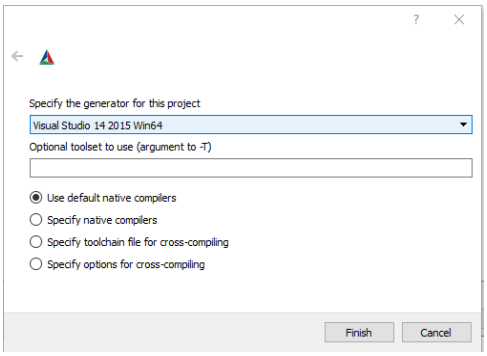
Starting from version `4.3.0` of CC3D the DeveloperZone compilation setup (for any compiler) is is done automatically. All you need to do is to follow procedure outlined in Configuring Developer Zone

After we generated plugin code and added our modification to those two files, we are ready to begin compilation. We will show how to compile code on Windows. Compilation on Linux system is analogous up to CMake configuration part but then instead of using Visual Studio you will type `make` and `make install` in the terminal. For now let's stick with Windows compilation. After Twedit++ generated new files in the `Developer Zone` we need to use CMake tool (GUI - as we will go here, or console based tool) to configure our compilation. This is how CMake configuration looks in our case



First we point to the folder where `DeveloperZone` is (`Where the source code is`). In our case it is `D:\CC3D_PY3_GIT\CompuCell3D\DeveloperZone` and location for our Visual Studio project `D:/CC3D_PY3_GIT_build_developer_zone` (see `Where to build the binaries`)

Then we after click `Configure` CMake will display the following dialog:

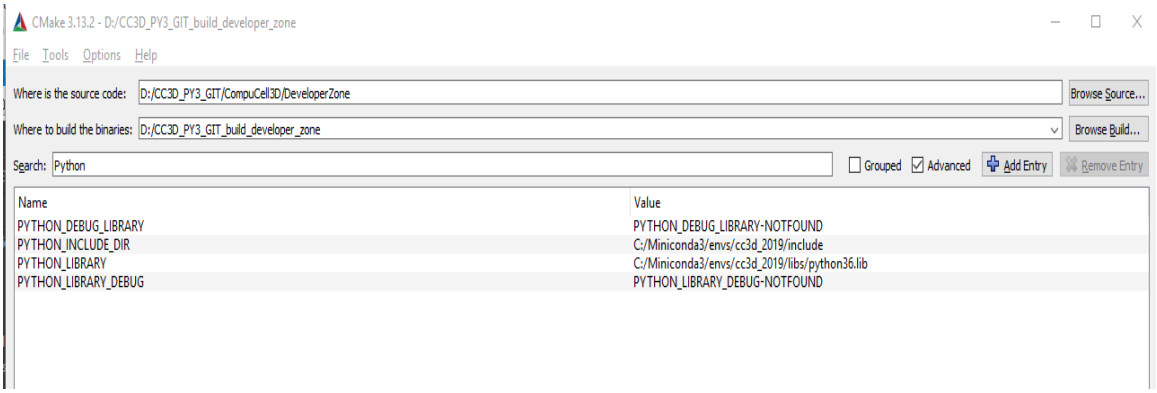


Make sure to select `Visual Studio 14 2015 Win64` (we assume we are using 64-bit version of CC3D). If you are using 32-bit version then you would select `Visual Studio 14 2015`

Next, we set `CMAKE_INSTALL_PREFIX` and `COMPUCELL3D_INSTALL_PATH` to the folder where CC3D is installed - `D:\Program Files\cc3d_py3_demo_new` .

We also set where main CC3D code-base is `COMPUCELL3D_FULL_SOURCE_PATH` `D:/CC3D_PY3_GIT/CompuCell3D/`

`core/CompuCell3D` Next, we set version number (*4*, *0*, *0*). We are almost done but since `DeveloperZone` also compiles Python module we must set Python paths as follows (you need to specify Python include directory and Python library path):



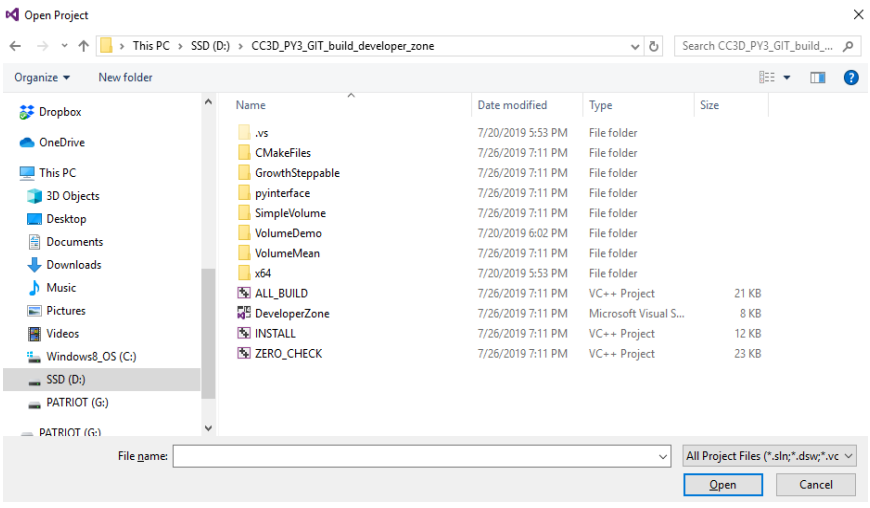
Note

It is perfectly fine to compile `DeveloperZone` modules without using Python. If this is what you would like to do, just comment out line `add_subdirectory(pyinterface)` in `DeveloperZone/CMakeLists.txt`

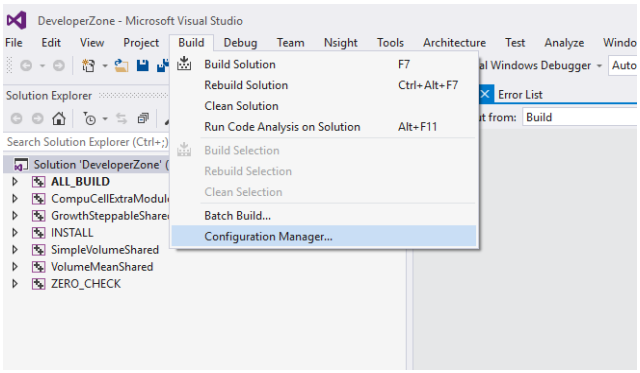
After we configured all paths in CMake GUI we press `Configure` button and then `Generate` button. The VisualStudio Project will be placed in `D:/CC3D_PY3_GIT_build_developer_zone` (see `Where to build the binaries` at the top of CMake GUI). We will open it next and will show you how to compile plugins and steppables in the `DeveloperZone`

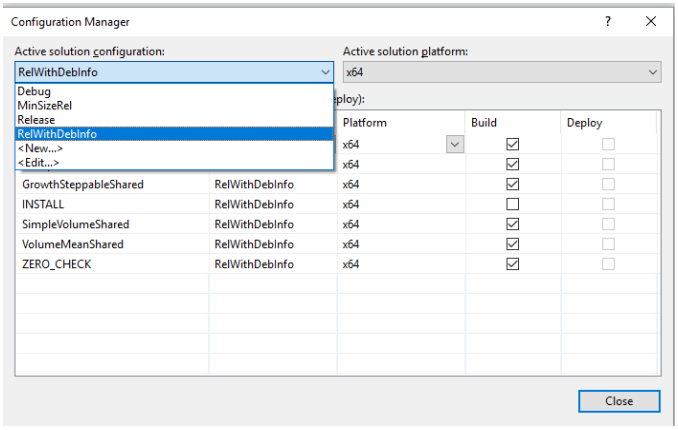
17.1 Compiling `DeveloperZone` in Visual Studio

Now that we created Visual Studio project for Developer Zone we will show you how to set up compilation. We open up Visual Studio and navigate to `File->Open->Project/Solution...` and in the File Open Dialog we go to `D:/CC3D_PY3_GIT_build_developer_zone` and select `ALL_BUILD.vcxproj`

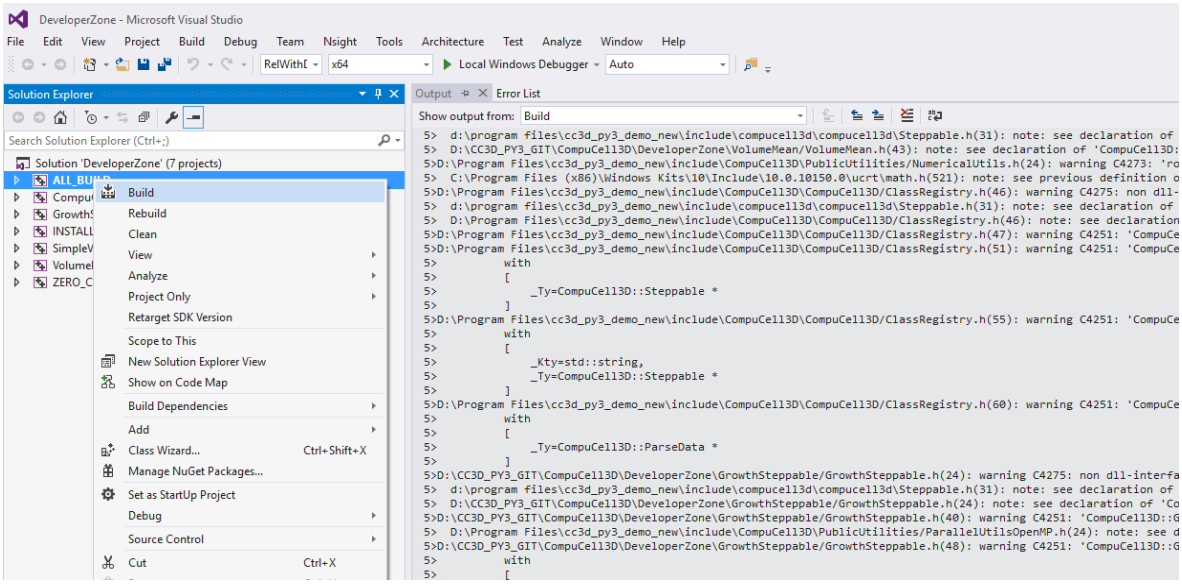


After `DeveloperZone` Visual Studio project gets loaded we go to `Build->Configuration Manager...` and from the pull down menu `Active Solution Configuration` (at the top of the dialog box) we select `RelWithDebInfo`:



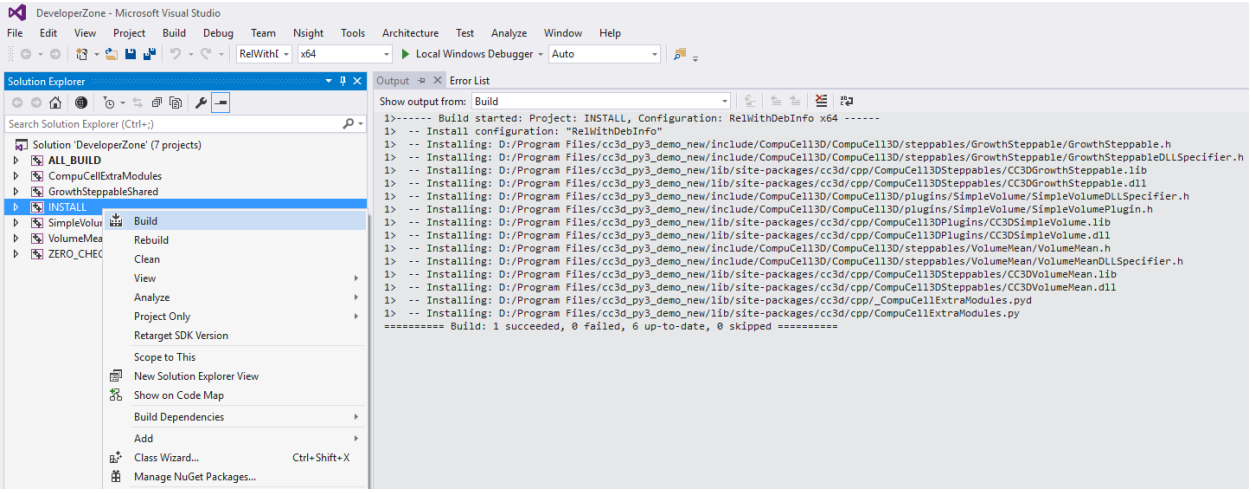


Next, to start compilation, we right-click on `ALL_BUILD` and from the context menu select `Build`:



Notice that there are additional modules in addition to our `GrowthSteppable`. Take a looks at those. They show how to write simple modules (plugins or steppables).

After the compilation finished and there are no errors, we right-click at `INSTALL` subproject and from the context menu we select `Build`. This will install our newly created `GrowthSteppable` in the CC3D installation directory that we specified during CMake configuration (`D:/Program Files/cc3d_py3_demo_new`)



At this point we can build a simulation that will use newly created `GrowthSteppable`

17.1.1 Using DeveloperZone steppable in the simulation

Writing C++ code and compiling it was a hard-part of the project. Using newly created steppable in the simulation is easy. In fact all we need to do is to add

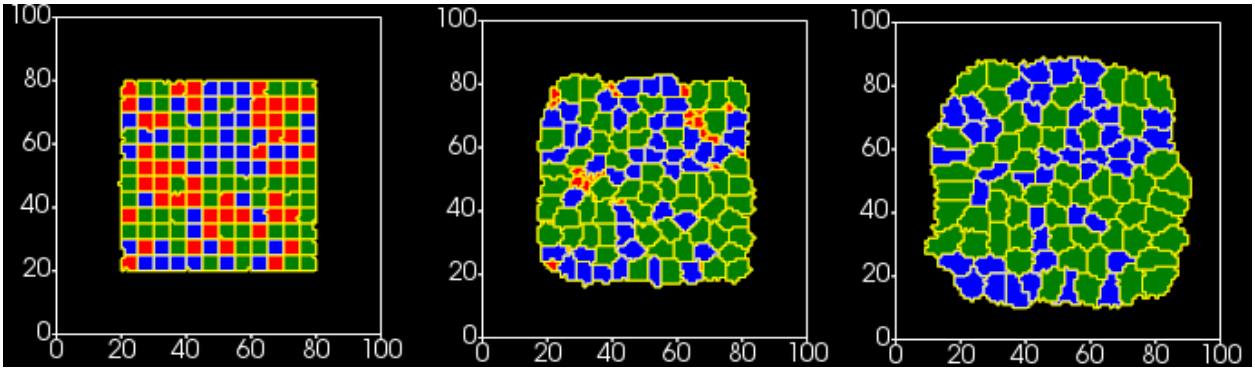
```
<Steppable Type="GrowthSteppable">
    <GrowthRate CellType="1" Rate="1.3"/>
    <GrowthRate CellType="2" Rate="1.7"/>
</Steppable>
```

to any simulation where we want cell of type *1* to increase target volume at 1.3 pixels/MCS rate and for cells of type 2 the growth would be 1.7.

Note

The name of the steppable or plugin that we reference from XML is not based on module name but on the label encoded in the proxy file. In our case `GrowthSteppableProxy.cpp` has the following line `growthSteppableProxy("GrowthSteppable", ...` and there we have label `GrowthSteppable` that we use in XML. If we changed this label to e.g. *growthSteppableProxy("MyGrowthSteppable", ...* ` then we would need to change first line of XML for GrowthSteppable to `<Steppable Type="GrowthSteppable">`

Here are the results of the simulation at MCS 0, 20, and 40:



As you can see there are 3 cell types here but we specified growth rates for two of them As a result "red" cells are

getting squashed by growing neighbors and at MCS 40 they disappear. Also notice that green cells are bigger than blue ones. This is what we expect when we have different growth rates.

Since we are modifying target volume we must use `Volume` plugin where we control all parameters for each cell individually - we use "local flex" version of Volume constraint `<Plugin Name="Volume"/>` where we only load `Volume` plugin but dont pass any parameters to it. Those parameters `targetVolume` `lambdaVolume` are set in C++ code:

```
<CompuCell3D Revision="20190604" Version="4.0.0">

   <Potts>

      <!-- Basic properties of CPM (GGH) algorithm -->
      <Dimensions x="100" y="100" z="1"/>
      <Steps>100000</Steps>
      <Temperature>10.0</Temperature>
      <NeighborOrder>1</NeighborOrder>
   </Potts>

   <Plugin Name="CellType">

      <!-- Listing all cell types in the simulation -->
      <CellType TypeId="0" TypeName="Medium"/>
      <CellType TypeId="1" TypeName="A"/>
      <CellType TypeId="2" TypeName="B"/>
      <CellType TypeId="3" TypeName="C"/>
   </Plugin>

   <Plugin Name="Volume"/>

   <Plugin Name="CenterOfMass">

      <!-- Module tracking center of mass of each cell -->
   </Plugin>

   <Plugin Name="Contact">
      <!-- Specification of adhesion energies -->
      <Energy Type1="Medium" Type2="Medium">10.0</Energy>
      <Energy Type1="Medium" Type2="A">10.0</Energy>
      <Energy Type1="Medium" Type2="B">10.0</Energy>
      <Energy Type1="Medium" Type2="C">10.0</Energy>
      <Energy Type1="A" Type2="A">10.0</Energy>
      <Energy Type1="A" Type2="B">10.0</Energy>
      <Energy Type1="A" Type2="C">10.0</Energy>
      <Energy Type1="B" Type2="B">10.0</Energy>
      <Energy Type1="B" Type2="C">10.0</Energy>
      <Energy Type1="C" Type2="C">10.0</Energy>
      <NeighborOrder>4</NeighborOrder>
   </Plugin>

   <Steppable Type="UniformInitializer">

      <!-- Initial layout of cells in the form of rectangular slab -->
      <Region>
```

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```
        <BoxMin x="20" y="20" z="0"/>
        <BoxMax x="80" y="80" z="1"/>
        <Gap>0</Gap>
        <Width>5</Width>
        <Types>A,B,C</Types>
      </Region>
   </Steppable>

    <Steppable Type="GrowthSteppable">
        <GrowthRate CellType="1" Rate="1.3"/>
        <GrowthRate CellType="2" Rate="1.7"/>
    </Steppable>

</CompuCell3D>
```

Note

We placed `GrowthSteppable` last. This is not coincidence. We must place it after steppable that creates cells `UniformInitializer`. If we reversed the order of those two steppables GrowthSteppable would be called first and in particular its `start` function would be called before `UniformInitializer` function and as a result the code that is supposed to set initaial volume constraint parameters from `GrowthSteppable` (`start` function) woudl iterate over empty cell inventory. Therefore, listing `UniformInitializer` before `GrowthSteppable` is the rihght thing to to. Simply put order of appearances of steppables in the XML determines the order in which CC3D will call them

Note

Specified growth rates of 1.3 and 1.7 are very high and we used them for illustration purposes. In your simulation you should much smaller rates to allow cells on the lattice to "equilibrate"

Full simulation can be downloaded here `zip` and full code for `GrowthSteppable` is here `zip`. You can also access both example and c++ code by going directly to `CompuCell3D/DeveloperZone`

CHAPTER

EIGHTEEN

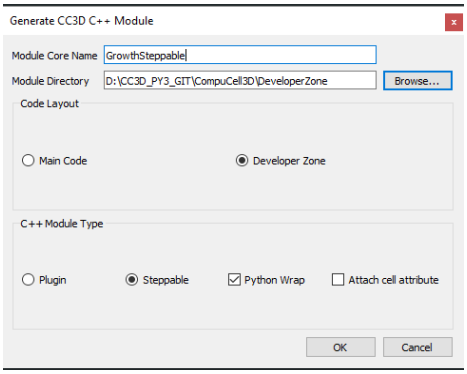
ADDING PYTHON BINDINGS TO STEPPABLE IN DEVELOPERZONE

In the previous example we controled entire simulation from C++. This is perfectly fine and will give you optimal performance. However sometimes it may make sense to add Python bindings to your module . Especially if the functions you wil call from python will not be called many times - functions calls in Python are much slower than in C++.

In addition to this if your entire code is in C++ every change you make to the code will require compilation and installation. This is is not a big deal but takes time and is more error prone than using well designed scripting interface. However, do not feel that you need to use Python bindings for your newly created C++ modules. They are optional and it is perfectly fine to operate in C++ space.

Nevertheless we would like to show you how to add and use Python bindings if you feel it will be beneficial for your simulation.

If you remember, the first step to generate steppable code using Twedit++ is to choose whether you like to add Python bindings or not.



In this first dialog box we checked `Python Wrap` option and therefore we already generated Python bindings. They are stored in SWIG file in `DeveloperZone/pyinterface/CompuCellExtraModules/CompuCellExtraModules.i`:

```
%module ("threads"=1) CompuCellExtraModules
%include "typemaps.i"
%include <windows.i>

%{
#include "ParseData.h"
#include "ParserStorage.h"
#include <CompuCell3D/Simulator.h>
#include <CompuCell3D/Potts3D/Potts3D.h>

#include <BasicUtils/BasicClassAccessor.h>
```

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```
#include <BasicUtils/BasicClassGroup.h> //had to include it to avoid problems with␣
↪template instantiation


// ********************************************* PUT YOUR PLUGIN PARSE DATA AND PLUGIN␣
↪FILES HERE ************************************************

#include <SimpleVolume/SimpleVolumePlugin.h>


#include <VolumeMean/VolumeMean.h>

//AutogeneratedModules1 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//GrowthSteppable_autogenerated


#include <GrowthSteppable/GrowthSteppable.h>



// ********************************************* END OF SECTION␣
↪*********************************  ***********************************************


//have to include all  export definitions for modules which are arapped to avoid␣
↪problems with interpreting by swig win32 specific c++ extensions...
#define SIMPLEVOLUME_EXPORT
#define VOLUMEMEAN_EXPORT
//AutogeneratedModules2 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//GrowthSteppable_autogenerated
#define GROWTHSTEPPABLE_EXPORT

#include <iostream>

using namespace std;
using namespace CompuCell3D;

%}

// C++ std::string handling
%include "std_string.i"

// C++ std::map handling
%include "std_map.i"

// C++ std::map handling
%include "std_set.i"

// C++ std::vector handling
%include "std_vector.i"
```

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```
//have to include all  export definitions for modules which are arapped to avoid␣
↪problems with interpreting by swig win32 specific c++ extensions...
#define SIMPLEVOLUME_EXPORT
#define VOLUMEMEAN_EXPORT

//AutogeneratedModules3 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//GrowthSteppable_autogenerated
#define GROWTHSTEPPABLE_EXPORT

%include <BasicUtils/BasicClassAccessor.h>
%include <BasicUtils/BasicClassGroup.h> //had to include it to avoid problems with␣
↪template instantiation

%include "ParseData.h"
%include "ParserStorage.h"

// ********************************************** PUT YOUR PLUGIN PARSE DATA AND PLUGIN␣
↪FILES HERE ***************************************************
// REMEMBER TO CHANGE #include to %include

%include <SimpleVolume/SimpleVolumePlugin.h>
// %include <SimpleVolume/SimpleVolumeParseData.h>

// THIS IS VERY IMORTANT STETEMENT WITHOUT IT SWIG will produce incorrect wrapper code␣
↪which will compile but will not work
using namespace CompuCell3D;

%inline %{
   SimpleVolumePlugin * reinterpretSimpleVolumePlugin(Plugin * _plugin){
      return (SimpleVolumePlugin *)_plugin;
   }

   SimpleVolumePlugin * getSimpleVolumePlugin(){
         return (SimpleVolumePlugin *)Simulator::pluginManager.get("SimpleVolume");
    }

%}

%include <VolumeMean/VolumeMean.h>

%inline %{
   VolumeMean * reinterpretVolumeMean(Steppable * _steppable){
      return (VolumeMean *)_steppable;
   }

   VolumeMean * getVolumeMeanSteppable(){
         return (VolumeMean *)Simulator::steppableManager.get("VolumeMean");
    }

%}
```

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```
//AutogeneratedModules4 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//GrowthSteppable_autogenerated

%include <GrowthSteppable/GrowthSteppable.h>
%inline %{

 GrowthSteppable * getGrowthSteppable(){

      return (GrowthSteppable *)Simulator::steppableManager.get("GrowthSteppable");
   }

%}
```

We are not going to explain how SWIG wrappers work here but if you look at the file and look for occurrences of `GrowthSteppable` you can see that adding your own steppable to the SWIG wrapper generator is fairly easy. On top of that if you use Twedit++ it will generate wrapper code for you.

Note

At the top of the wrapper file we find `%module ("threads"=1) CompuCellExtraModules` . This tells us that the Python module we develop will be called `CompuCellExtraModules`.

18.1 Adding Python-Accessible Method To GrowthSteppable

If we enable compilation of `CompuCellExtraModules` by uncommenting line `add_subdirectory(pyinterface)` in `DeveloperZone/CMakeLists.txt` we will already get GrowthSteppable bindings that we can access from `CompuCellExtraModules`. However, they are not particularly useful because all the functions accessible via Python are for functions that are already being used by the C++ code and, frankly it is best to leave it like that. We need to add additional function. A reasonable choice is a function that changes growth rate for a given cell type.

First we need to add `void setGrowthRate(unsigned int cellType, double growthRate); `` function to ``GrowthSteppable` header - see below:

```
#ifndef GROWTHSTEPPABLESTEPPABLE_H
#define GROWTHSTEPPABLESTEPPABLE_H
#include <CompuCell3D/CC3D.h>
#include "GrowthSteppableDLLSpecifier.h"

namespace CompuCell3D {

    template <class T> class Field3D;
    template <class T> class WatchableField3D;

    class Potts3D;
    class Automaton;
    class BoundaryStrategy;
    class CellInventory;
    class CellG;
```

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```
class GROWTHSTEPPABLE_EXPORT GrowthSteppable : public Steppable {

  WatchableField3D<CellG *> *cellFieldG;

  Simulator * sim;

  Potts3D *potts;

  CC3DXMLElement *xmlData;

  Automaton *automaton;

  BoundaryStrategy *boundaryStrategy;

  CellInventory * cellInventoryPtr;

  Dim3D fieldDim;

public:

  GrowthSteppable ();

  virtual ~GrowthSteppable ();

  std::map<unsigned int, double> growthRateMap;

  // SimObject interface

  virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);

  virtual void extraInit(Simulator *simulator);

  // Python wrapper functions

  void setGrowthRate(unsigned int cellType, double growthRate);

  //steppable interface

  virtual void start();

  virtual void step(const unsigned int currentStep);

  virtual void finish() {}


  //SteerableObject interface

  virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false);

  virtual std::string steerableName();

  virtual std::string toString();
```

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```
  };

};

#endif
```

Next, we add implementation of this function in the `GrowthSteppable.cpp`:

```
void GrowthSteppable::setGrowthRate(unsigned int cellType, double growthRate){

    cerr<<"CHANGING GROWTH RATE FOR CELL TYPE "<<cellType<<" TO "<<growthRate<<endl;
    this->growthRateMap[cellType] = growthRate;
}
```

The implementation of this function is pretty straightforward - it is a function that takes two arguments `(unsigned int cellType` and `double growthRate` and prints out message to the screen that it is about to change growth rate for a given cell type and then assigns a growth rate to a given entry in the `this->growthRateMap`.

Why does this function make sense to be implemented in Python? If you think about a simulation where you want to run many simulations that need to modify growth rate at a particular MCS but you don't know which MCS it will be you can write a simple code where you could try many time points at this you change growth rate and see if the outcome matches your expectations. Obviously, you could do it all in c++ but then you would need to pass more parameters to the XML making XML harder and harder to understand or you could hard-code everything in C++ but then you would need to recompile DeveloperZone every time you run the simulation. You quickly realize that Python provides convenient platform for handling situations like this. This is why , it makes perfect sense to add Python bindings to your C++ modules.

At this point we can recompile the DeveloperZone but before we do it it is essential that we "touch" `DeveloperZone/pyinterface/CompuCellExtraModules/CompuCellExtraModules.i` by e.g. add or remove empty line in this file and re-saving it.

> **Warning**
>
> If you add new method to header file and want this method be accessible in Python bindings you must force SWIG to re-generate bindings. One way of doing so is by "refreshing" the file but making adding (or removing) extra empty line and saving it. In the future we will write better CMake code to avoid this manual step but for now you should be aware of this limitation.

After we compiled and installed `DeveloperZone` modules we can rerun the simulation. Now, however, we will add Python code where we show you how to access new C++ steppable from Python.

Here is python Steppable code (`GrowthSteppablePythonModules`):

```
from cc3d.core.PySteppables import *
from cc3d.cpp import CompuCellExtraModules

class GrowthSteppablePython(SteppableBasePy):

    def __init__(self,frequency=1):

        SteppableBasePy.__init__(self,frequency)
        self.growth_steppable_cpp = None
```

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```
    def start(self):
        self.growth_steppable_cpp = CompuCellExtraModules.getGrowthSteppable()

    def step(self,mcs):

        if mcs == 10:
            self.growth_steppable_cpp.setGrowthRate(1, -1.2)
```

At the top of the file we import `CompuCellExtraModules`. This is the module that SWIG generated for us In `__init__` constructor we create a variable that will hold a reference to the C++ `GrowthSteppable`. In start function we access C++ `GrowthSteppable` by typing:

```
self.growth_steppable_cpp = CompuCellExtraModules.getGrowthSteppable()
```

If you look at the end of the `DeveloperZone/pyinterface/CompuCellExtraModules/CompuCellExtraModules.i` you will see `getGrowthSteppable()` declared there. In other words `getGrowthSteppable()` function will become a function of the `CompuCellExtraModules` and therefore we access it as `CompuCellExtraModules.getGrowthSteppable()`. Now, we can get creative, because we can access every publicly defined function of the C++ `GrowthSteppable`. This is exactly what we do in the `step` function. We call our newly added function

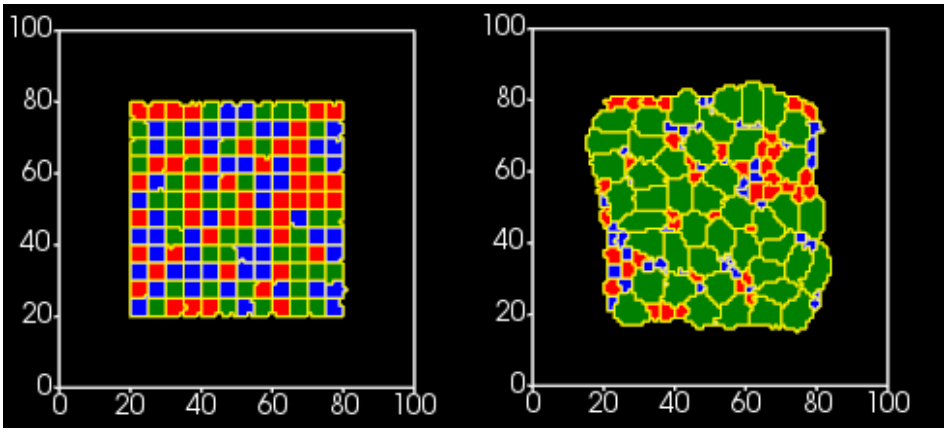
```
self.growth_steppable_cpp.setGrowthRate(1, -1.2)
```

This call at MCS=10 changes growth of cells of type *1* into shrinking rate.

When we run the simulation at `mcs==10` the text output will look as follows:

```
total number of pixel copy attempts=10000
Number of Attempted Energy Calculations=910
Step 8 Flips 210/10000 Energy -803.2 Cells 144 Inventory=144
Metropolis Fast
total number of pixel copy attempts=10000
Number of Attempted Energy Calculations=870
Step 9 Flips 236/10000 Energy -1074.4 Cells 144 Inventory=144
Metropolis Fast
total number of pixel copy attempts=10000
Number of Attempted Energy Calculations=859
Step 10 Flips 236/10000 Energy -1244 Cells 144 Inventory=144
CHANGING GROWTH RATE FOR CELL TYPE 1 TO -1.2
```

You can see there our C++ printout being triggered by calling `setGrowthRate` from Python level. And the simulation configuration at MCS 0 and 30 respectively will looks as follows:



Notice that the blue cells almost disappeared. This is the result of the negative growth rate we we set by calling `self.growth_steppable_cpp.setGrowthRate(1, -1.2)` .

The C++ code for this example can be found in `DeveloperZone/GrowthSteppable`, python bindings are in `DeveloperZone/pyinterface/CompuCellExtraModules/CompuCellExtraModules.i` and the simulation example is in `CompuCell3D/DeveloperZone/Demos/GrowthSteppablePython`

CHAPTER

NINETEEN

COMPUTING HETEROTYPIC BOUNDARY LENGTH

Heterotypic boundary surface (or length in 2D) is total surface of contact between all cells of two types. For example when you have 2 cells of type *1* and 100 cells of type *2* the heterotypic surface between thw two will be a sum of all contact surfaces between the two types. In this example we are not going to show every step how we generate the steppable using Twedit. We have shown this earlier and here we will concentrate on the actual code.

This example is a bit more advanced but we will explain clearly every line of code.

The module that we generated is called `HeterotypicBoundaryLength`. We then click `Configure` and `Generate` in the CMake Gui and start writing actual code. We will first implement function that walks over entire lattice and computes heterotypic surface (or length in 2D) between all cells of different types.

All C++ files can be found in `DeveloperZone/Demos/HeterotypicBoundarySurface` and Python bindings are , as usual in `DeveloperZone/pyinterface/CompuCellExtraModules/CompuCellExtraModules.i`. The simulation example that uses our newly created module is in `DeveloperZone/Demos/HeterotypicBoundarySurface`

Here is the header file for our new steppable:

```
#ifndef HETEROTYPICBOUNDARYLENGTHSTEPPABLE_H
#define HETEROTYPICBOUNDARYLENGTHSTEPPABLE_H
#include <CompuCell3D/CC3D.h>
#include "HeterotypicBoundaryLengthDLLSpecifier.h"

namespace CompuCell3D {

  template <class T> class Field3D;
  template <class T> class WatchableField3D;

    class Potts3D;
    class Automaton;
    class BoundaryStrategy;
    class CellInventory;
    class CellG;

  class HETEROTYPICBOUNDARYLENGTH_EXPORT HeterotypicBoundaryLength : public Steppable {

    WatchableField3D<CellG *> *cellFieldG;

    Simulator * sim;
    Potts3D *potts;
    CC3DXMLElement *xmlData;
    Automaton *automaton;
    BoundaryStrategy *boundaryStrategy;
```

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```
    CellInventory * cellInventoryPtr;
    Dim3D fieldDim;

  public:

    HeterotypicBoundaryLength ();

    virtual ~HeterotypicBoundaryLength ();

    // new methods and members

    std::map<unsigned int, double> typePairHTSurfaceMap;

    unsigned int typePairIndex(unsigned int cellType1, unsigned int cellType2);
    void calculateHeterotypicSurface();
    double getHeterotypicSurface(unsigned int cellType1, unsigned int cellType2);

    // SimObject interface

    virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);

    virtual void extraInit(Simulator *simulator);

    //steppable interface

    virtual void start();

    virtual void step(const unsigned int currentStep);

    virtual void finish() {}

    //SteerableObject interface

    virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false);

    virtual std::string steerableName();

     virtual std::string toString();


  };

};

#endif
```

we added few methods and one class member there:

```
// new methods and members

std::map<unsigned int, double> typePairHTSurfaceMap;
```

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```
unsigned int typePairIndex(unsigned int cellType1, unsigned int cellType2);
void calculateHeterotypicSurface();
double getHeterotypicSurface(unsigned int cellType1, unsigned int cellType2);
```

The typePairHTSurfaceMap is a dictionary (map) that will store heterotypic boundary surface between different cell types. Notice that we will encode pair of cell types as a single unsigned integer (hence a key to the dictionary is unsigned integer). To do this we will use convenience function `unsigned int typePairIndex(unsigned int cellType1, unsigned int cellType2)` that takes as its arguments two unsigned integers that denote cell type 1 and cell type 2. Here is the implementation of this function:

```
unsigned int HeterotypicBoundaryLength::typePairIndex(unsigned int cellType1, unsigned␣
↪int cellType2) {
    return 256 * cellType2 + cellType1;
}
```

we take advantage of the fact that the number of cell types in CC3D is limited to 256 and the index this function returns looks analogous to the index you woudl use to access a matrix if you were to store a matrix as 1D array.

Next we have two functions `calculateHeterotypicSurface()` that computed actual total heterotypic surface between all cell types and `double getHeterotypicSurface(unsigned int cellType1, unsigned int cellType2)` that given two types it returns a boundary between them.

Let's start analyzing code for `calculateHeterotypicSurface` function:

```
1  void HeterotypicBoundaryLength::calculateHeterotypicSurface() {
2
3      unsigned int maxNeighborIndex = this->boundaryStrategy->
   ↪getMaxNeighborIndexFromNeighborOrder(1);
4      Neighbor neighbor;
5
6      CellG *nCell = 0;
7
8      this->typePairHTSurfaceMap.clear();
9
10     // note: unit surface is different on a hex lattice. if you are runnign
11     // this steppable on hex lattice you need to adjust it. Remember that on hex lattice␣
   ↪unit length and unit surface have different values
12     double unit_surface = 1.0;
13
14     cerr << "Calculating HTBL for all cell type combinations" << endl;
15
16     for (unsigned int x = 0; x < fieldDim.x; ++x)
17         for (unsigned int y = 0; y < fieldDim.y; ++y)
18             for (unsigned int z = 0; z < fieldDim.z; ++z) {
19                 Point3D pt(x, y, z);
20                 CellG *cell = this->cellFieldG->get(pt);
21
22                 unsigned int cell_type = 0;
23                 if (cell) {
24                     cell_type = (unsigned int)cell->type;
25                 }
26
27                 for (unsigned int nIdx = 0; nIdx <= maxNeighborIndex; ++nIdx) {
```

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```
28                      neighbor = boundaryStrategy->getNeighborDirect(const_cast<Point3D&>
↪(pt), nIdx);
29                      if (!neighbor.distance) {
30                          //if distance is 0 then the neighbor returned is invalid
31                          continue;
32                      }
33
34                      nCell = this->cellFieldG->get(neighbor.pt);
35                      unsigned int n_cell_type = 0;
36                      if (nCell) {
37                          n_cell_type = (unsigned int)nCell->type;
38                      }
39
40                      if (nCell != cell) {
41                          unsigned int pair_index_1 = typePairIndex(cell_type, n_cell_
↪type);
42                          unsigned int pair_index_2 = typePairIndex(n_cell_type, cell_
↪type);
43                          this->typePairHTSurfaceMap[pair_index_1] += unit_surface;
44                          if (pair_index_1 != pair_index_2) {
45                              this->typePairHTSurfaceMap[pair_index_2] += unit_surface;
46                          }
47
48                      }
49
50                  }
51
52              }
53
54  }
```

We will be iterating over lattice pixels. Every lattice pixel has neighbors of different order but 1-st order neighbors are simply adjacent pixels. `BoundaryStrategy` is an object that facilitates iteration over pixel neighbors and it also keeps track of boundary conditions, pixels, adjacent to the boundary etc. so that you can write a simpler code. All we need to do to iterate over 1-st order pixel neighbors is to know what is the maximum number of them and this is what we do in this line:

```
unsigned int maxNeighborIndex = this->boundaryStrategy->
↪getMaxNeighborIndexFromNeighborOrder(1);
```

We get maximum index of a 1-st order pixel (`BoundaryStrategy` keeps them in a vector and we are getting max index of this vector). On 2D. cartesian lattice there could be up to 4 such neighbors hence the max vector index is 3 (we start counting from 0).

We next clear the map where we store our results because each time we call this function it wil be incrementing the values so if we did not clear we would be starting counting from different value that zero.

At line 16 we start triple loop where we iterate over all lattice pixels. This might not be the most efficient method but it is the simplest to code.

In lines 19 and 20 we get a cell that resides at a given pixel. If the cell pointer returned is `NULL` we are dealing with `Medium` and cell and this is why in lines 23-25 we check if the cell is different than `NULL` (`if (cell)`) before accessing its type. If it is null that we do not execute line 24 and the cell type is 0 as it should be for the Medium.

At line 27 we start iterating over neighbors of the current pixel (`Point3D pt(x, y, z)`). This is where we do actual

calculations. Code in line 28 fetches one of the neighbor of pixel `pt(x, y, z)`. In line 30 we check if this neighbor is a valid one (e.g. if you are at the edge of the lattice we may get pixel that is outside of the lattice and then if `neighbor.distance` is zero we know we are dealing with invalid pixel), hence in the line 31 we skip the rest of the loop. If, however, the pixel is valid then we get a cell that resides at the neighboring pixel (line 34):

```
nCell = this->cellFieldG->get(neighbor.pt);
```

In lines 35-38 we extract cell type of neighbor cell , again we have to be mindful of `Medium` as we did in lines 22-25.

Finally, lines 41-45 contain actual code that increments boundary surface between two cell types. This code runs only if `nCell` and `cell` *i.e.* cells belonging to adjacent pixels are different cells. In this case we compute index for type of `nCell` and type of `cell` (`unsigned int pair_index_1 = typePairIndex(cell_type, n_cell_type);`)

and increment appropriate entry in the `this->typePairHTSurfaceMap` - lines 43. Notice that we also permute cell types in call to `typePairIndex` - line 44-45. so that when we access boundary length between cell type 1 and 2 it will give us the same value as between cell types 2 and 1. But we do this only when the two types are different

Obviously, we are double-counting and we correct this in the function that returns heterotypic surfaces:

```
double HeterotypicBoundaryLength::getHeterotypicSurface(unsigned int cellType1, unsigned␣
↪int cellType2) {
    unsigned int pair_index = typePairIndex(cellType1, cellType2);

    double heterotypic_surface = this->typePairHTSurfaceMap[pair_index]/2.0;

    return heterotypic_surface;
}
```

19.1 Running the Simulation with Heterotypic Surface Calculator

The simulation code is quite easy to write as it follows the same pattern that we encountered in the previous chapter where we introduced Python bindings to the C++ steppable. We start with an XML file:

```
1  <CompuCell3D Revision="20190604" Version="4.0.0">
2     <Potts>
3        <!-- Basic properties of CPM (GGH) algorithm -->
4        <Dimensions x="256" y="256" z="1"/>
5        <Steps>100000</Steps>
6        <Temperature>10.0</Temperature>
7        <NeighborOrder>1</NeighborOrder>
8     </Potts>
9
10    <Plugin Name="CellType">
11       <!-- Listing all cell types in the simulation -->
12       <CellType TypeId="0" TypeName="Medium"/>
13       <CellType TypeId="1" TypeName="A"/>
14       <CellType TypeId="2" TypeName="B"/>
15    </Plugin>
16
17    <Plugin Name="Volume">
18       <VolumeEnergyParameters CellType="A" LambdaVolume="2.0" TargetVolume="50"/>
19       <VolumeEnergyParameters CellType="B" LambdaVolume="2.0" TargetVolume="50"/>
20    </Plugin>
21
```

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```
22    <Plugin Name="CenterOfMass">
23       <!-- Module tracking center of mass of each cell -->
24    </Plugin>
25
26    <Plugin Name="Contact">
27       <!-- Specification of adhesion energies -->
28       <Energy Type1="Medium" Type2="Medium">10.0</Energy>
29       <Energy Type1="Medium" Type2="A">10.0</Energy>
30       <Energy Type1="Medium" Type2="B">10.0</Energy>
31       <Energy Type1="A" Type2="A">10.0</Energy>
32       <Energy Type1="A" Type2="B">10.0</Energy>
33       <Energy Type1="B" Type2="B">10.0</Energy>
34       <NeighborOrder>4</NeighborOrder>
35    </Plugin>
36
37    <Steppable Type="UniformInitializer">
38       <!-- Initial layout of cells in the form of rectangular slab -->
39       <Region>
40          <BoxMin x="51" y="51" z="0"/>
41          <BoxMax x="204" y="204" z="1"/>
42          <Gap>0</Gap>
43          <Width>7</Width>
44          <Types>A,B</Types>
45       </Region>
46    </Steppable>
47
48    <Steppable Type="HeterotypicBoundaryLength"/>
49
50 </CompuCell3D>
```

It is Twedit-generated XML file that has basic energy terms (Volume and Contact Constraints) plus initializer and at the end in line 48 we add our new `HeterotypicBoundaryLength` steppable. Notice that this is a one-line call because we are not really passing any parameters to the steppable from the XML and our `update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false)` method does not contain any code that parses XML.

Note

It is important that every module (steppable, plugin) that you develop in C++ be instantiated in XML. Otherwise it will not be loaded and you will not be able to use it from Python. You can, however, write Python code that will properly load and initialize your module but this approach is way more complex than adding a simple line or lines in the XML.

In our example even if we add `<Steppable Type="HeterotypicBoundaryLength"/>` to the XML we will not see any calculations being done. Why? Because `start` and `step` functions are empty:

```
void HeterotypicBoundaryLength::start(){
}

void HeterotypicBoundaryLength::step(const unsigned int currentStep){
}
```

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```
void HeterotypicBoundaryLength::update(CC3DXMLElement *_xmlData, bool _fullInitFlag){

    //PARSE XML IN THIS FUNCTION

    //For more information on XML parser function please see CC3D code or lookup XML␣
↪utils API

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)

    //boundaryStrategy has information about pixel neighbors
    boundaryStrategy=BoundaryStrategy::getInstance();

}
```

We left those implementations empty on purpose. We wanted to show you how you can use steppable to implement functionality that gets called on-demand from Python code. Let us now look at the Python code:

```
1  from cc3d.core.PySteppables import *
2  from cc3d.cpp import CompuCellExtraModules
3
4
5  class HeterotypicBoundarySurfaceSteppable(SteppableBasePy):
6
7      def __init__(self, frequency=1):
8          SteppableBasePy.__init__(self, frequency)
9          self.htbl_steppable_cpp = None
10
11     def start(self):
12         self.htbl_steppable_cpp = CompuCellExtraModules.getHeterotypicBoundaryLength()
13
14     def step(self, mcs):
15         self.htbl_steppable_cpp.calculateHeterotypicSurface()
16
17         print(' HTBL between type 1 and 2 is ',
18               self.htbl_steppable_cpp.getHeterotypicSurface(1, 2))
19
20         print(' HTBL between type 2 and 1 is ',
21               self.htbl_steppable_cpp.getHeterotypicSurface(1, 2))
22
23         print(' HTBL between type 1 and 1 is ',
24               self.htbl_steppable_cpp.getHeterotypicSurface(1, 1))
25
26         print(' HTBL between type 0 and 1 is ',
27               self.htbl_steppable_cpp.getHeterotypicSurface(0, 1))
28
29         print('THIS ENTRY DOES NOT EXIST. HTBL between type 3 and 20 is ',
30               self.htbl_steppable_cpp.getHeterotypicSurface(3, 20))
```

At the top we import `CompuCellExtraModules` that SWIG generates. This Python contains contains Python-wrapper for our `HeterotypicBoundaryLength` C++ steppable. In line 12 we fetch a reference to the steppable and store it in

class-accessible `self.htbl_steppable_cpp` variable. In Python steppable `step` function we call C++ function that calculates heterotypic surface (line 15). The next series of `print` statements fetches results fo the calculations - see lines 18 21, *etc.*. . . . The output looks as follows:

```
Calculating HTBL for all cell type combinations
 HTBL between type 1 and 2 is  3261.0
 HTBL between type 2 and 1 is  3261.0
 HTBL between type 1 and 1 is  1804.0
 HTBL between type 0 and 1 is  321.0
THIS ENTRY DOES NOT EXIST. HTBL between type 3 and 20 is  0.0
Metropolis Fast
total number of pixel copy attempts=65536
Number of Attempted Energy Calculations=3640
Step 2 Flips 367/65536 Energy 1300 Cells 484 Inventory=484
Calculating HTBL for all cell type combinations
 HTBL between type 1 and 2 is  3268.0
 HTBL between type 2 and 1 is  3268.0
 HTBL between type 1 and 1 is  1814.0
 HTBL between type 0 and 1 is  326.0
THIS ENTRY DOES NOT EXIST. HTBL between type 3 and 20 is  0.0
```

Note that heterotypic surface between types 1 and 2 is the same as between 2 and 1. This is why, earlier in the C++ code we included two pair indexes:

```
unsigned int pair_index_1 = typePairIndex(cell_type, n_cell_type);
unsigned int pair_index_2 = typePairIndex(n_cell_type, cell_type);
```

Notice also that if we try to access heterotypic surface between types 3 and 20 (none of those types exist in our simulation) we get back `0.0`. Why? The answer has to do with the behavior of C++ `std::map` container. If we try to use a key that does not exist in the map the C++ will add this key and initialize the value of the key value-pair to the whatever default constructor of the value type is. In our case our map container has the following type : `std::map<unsigned int, double> typePairHTSurfaceMap` so that key is of `unsigned int` type and value is of `double` type. Any modern C++ compiler will put `0.0` as a default value for objects of type `double`. If you are familiar with Python `defaultdict` class that is a member of standard `collections` package than you can see similarities. C++ `std::map` behaves in similar way to the `defaultdict` Therefore when we access `typePairHTSurfaceMap` using key that does not exist C++ will insert this key into `typePairHTSurfaceMap` and set value to `0.0`. This is also a reason why the following code works at all:

```
this->typePairHTSurfaceMap[pair_index_1] += unit_surface
```

This brings us to the last remark we want to make regarding the C++ code. Why are we using `unit_surface` and not 1.0? It has to do with various lattices that CC3D supports. For Cartesian 2D or 3D lattice unit surface has value 1.0. However, hexagonal lattices are constructed in such a way that the volume of a voxel is constrained to be 1.0. Therefore from geometry constraints it follows that in 2D on hex lattice unit surface (or length) is `sqrt(2.0 / (3.0*sqrt(3.0)))` which is approx equal to `0.6204` and in 3D it is `8.0 / 12.0*sqrt(2.0)*pow(9.0 / (16.0*sqrt(3.0)), 1.0 / 3.0)*pow(9.0 / (16.0*sqrt(3.0)), 1.0 / 3.0)` which is approx equal to `0.445`

For more information please see http://www.compucell3d.org/BinDoc/cc3d_binaries/Manuals/HexagonalLattice.pdf as well as in the code of the BoundaryStrategy class method `LatticeMultiplicativeFactors BoundaryStrategy::generateLatticeMultiplicativeFactors(LatticeType _latticeType, Dim3D dim)` in `CompuCell3D/core/CompuCell3D/Boundary/BoundaryStrategy.cpp`

For completeness we also show SWIG file that was used to generate the wrapper :

```
%module ("threads"=1) CompuCellExtraModules

%include "typemaps.i"

%include <windows.i>

%{

#include "ParseData.h"
#include "ParserStorage.h"
#include <CompuCell3D/Simulator.h>
#include <CompuCell3D/Potts3D/Potts3D.h>

#include <BasicUtils/BasicClassAccessor.h>
#include <BasicUtils/BasicClassGroup.h> //had to include it to avoid problems with␣
↪template instantiation


// ********************************************* PUT YOUR PLUGIN PARSE DATA AND PLUGIN␣
↪FILES HERE ************************************************

#include <SimpleVolume/SimpleVolumePlugin.h>
#include <VolumeMean/VolumeMean.h>

//AutogeneratedModules1 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//HeterotypicBoundaryLength_autogenerated

#include <HeterotypicBoundaryLength/HeterotypicBoundaryLength.h>

//GrowthSteppable_autogenerated

#include <GrowthSteppable/GrowthSteppable.h>


// ********************************************* END OF SECTION␣
↪*********************************** ************************************************


//have to include all  export definitions for modules which are arapped to avoid␣
↪problems with interpreting by swig win32 specific c++ extensions...
#define SIMPLEVOLUME_EXPORT
#define VOLUMEMEAN_EXPORT
//AutogeneratedModules2 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//HeterotypicBoundaryLength_autogenerated
#define HETEROTYPICBOUNDARYLENGTH_EXPORT
//GrowthSteppable_autogenerated
#define GROWTHSTEPPABLE_EXPORT

#include <iostream>

using namespace std;
```

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```
using namespace CompuCell3D;

%}

// C++ std::string handling
%include "std_string.i"

// C++ std::map handling
%include "std_map.i"

// C++ std::map handling
%include "std_set.i"

// C++ std::vector handling
%include "std_vector.i"

//have to include all  export definitions for modules which are arapped to avoid␣
↪problems with interpreting by swig win32 specific c++ extensions...
#define SIMPLEVOLUME_EXPORT
#define VOLUMEMEAN_EXPORT

//AutogeneratedModules3 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//HeterotypicBoundaryLength_autogenerated
#define HETEROTYPICBOUNDARYLENGTH_EXPORT
//GrowthSteppable_autogenerated
#define GROWTHSTEPPABLE_EXPORT

%include <BasicUtils/BasicClassAccessor.h>
%include <BasicUtils/BasicClassGroup.h> //had to include it to avoid problems with␣
↪template instantiation
%include "ParseData.h"
%include "ParserStorage.h"


// ********************************************* PUT YOUR PLUGIN PARSE DATA AND PLUGIN␣
↪FILES HERE ***************************************************
// REMEMBER TO CHANGE #include to %include
%include <SimpleVolume/SimpleVolumePlugin.h>
// %include <SimpleVolume/SimpleVolumeParseData.h>
// THIS IS VERY IMORTANT STETEMENT WITHOUT IT SWIG will produce incorrect wrapper code␣
↪which will compile but will not work
using namespace CompuCell3D;

%inline %{
   SimpleVolumePlugin * reinterpretSimpleVolumePlugin(Plugin * _plugin){
      return (SimpleVolumePlugin *)_plugin;
   }

   SimpleVolumePlugin * getSimpleVolumePlugin(){
         return (SimpleVolumePlugin *)Simulator::pluginManager.get("SimpleVolume");
    }
```

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```
%}

%include <VolumeMean/VolumeMean.h>

%inline %{
   VolumeMean * reinterpretVolumeMean(Steppable * _steppable){
      return (VolumeMean *)_steppable;
   }

   VolumeMean * getVolumeMeanSteppable(){
         return (VolumeMean *)Simulator::steppableManager.get("VolumeMean");
    }
%}

//AutogeneratedModules4 - DO NOT REMOVE THIS LINE IT IS USED BY TWEDIT TO LOCATE CODE␣
↪INSERTION POINT
//HeterotypicBoundaryLength_autogenerated
%include <HeterotypicBoundaryLength/HeterotypicBoundaryLength.h>
%inline %{

 HeterotypicBoundaryLength * getHeterotypicBoundaryLength(){
      return (HeterotypicBoundaryLength *)Simulator::steppableManager.get(
↪"HeterotypicBoundaryLength");
   }
%}

//GrowthSteppable_autogenerated
%include <GrowthSteppable/GrowthSteppable.h>
%inline %{

 GrowthSteppable * getGrowthSteppable(){
      return (GrowthSteppable *)Simulator::steppableManager.get("GrowthSteppable");
   }
%}

// ********************************************* END OF SECTION␣
↪********************************** *********************************************
```

CHAPTER

TWENTY

ATTACHING CUSTOM ATTRIBUTES TO CELLS

Cells in CompuCell3D are represented by `CellG` class - see `CompuCell3D/core/CompuCell3D/Potts3D/Cell.h`

```
#ifndef CELL_H
#define CELL_H


#ifndef PyObject_HEAD
struct _object; //forward declare
typedef _object PyObject; //type redefinition
#endif

class BasicClassGroup;

namespace CompuCell3D {

  /**
   * A Potts3D cell.
   */

   class CellG{
   public:
      typedef unsigned char CellType_t;
      CellG():
        volume(0),
        targetVolume(0.0),
        lambdaVolume(0.0),
        surface(0),
        targetSurface(0.0),
        lambdaSurface(0.0),
        clusterSurface(0.0),
        targetClusterSurface(0.0),
        lambdaClusterSurface(0.0),
        type(0),
        xCM(0),yCM(0),zCM(0),
        xCOM(0),yCOM(0),zCOM(0),
        xCOMPrev(0),yCOMPrev(0),zCOMPrev(0),
        iXX(0), iXY(0), iXZ(0), iYY(0), iYZ(0), iZZ(0),
        lX(0.0),
        lY(0.0),
        lZ(0.0),
```

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```
        lambdaVecX(0.0),
        lambdaVecY(0.0),
        lambdaVecZ(0.0),
        flag(0),
        id(0),
        clusterId(0),
        fluctAmpl(-1.0),
        lambdaMotility(0.0),
        biasVecX(0.0),
        biasVecY(0.0),
        biasVecZ(0.0),
        connectivityOn(false),
        extraAttribPtr(0),
        pyAttrib(0)


     {}
     long volume;
     float targetVolume;
     float lambdaVolume;
     double surface;
     float targetSurface;
     float angle;
     float lambdaSurface;
     double clusterSurface;
     float targetClusterSurface;
     float lambdaClusterSurface;
     unsigned char type;
     unsigned char subtype;
     double xCM,yCM,zCM; // numerator of center of mass expression (components)
     double xCOM,yCOM,zCOM; // numerator of center of mass expression (components)
     double xCOMPrev,yCOMPrev,zCOMPrev; // previous center of mass
     double iXX, iXY, iXZ, iYY, iYZ, iZZ; // tensor of inertia components
     float lX,lY,lZ; //orientation vector components - set by MomentsOfInertia Plugin -␣
↪read only
     float ecc; // cell eccentricity
     float lambdaVecX,lambdaVecY,lambdaVecZ; // external potential lambda vector␣
↪components
     unsigned char flag;
     float averageConcentration;
     long id;
     long clusterId;
     double fluctAmpl;
     double lambdaMotility;
     double biasVecX;
     double biasVecY;
     double biasVecZ;
     bool connectivityOn;
     BasicClassGroup *extraAttribPtr;

     PyObject *pyAttrib;
  };
```

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```
  class Cell {
  };

  class CellPtr{
   public:
   Cell * cellPtr;
  };
};
#endif
```

As you can see CellG has a number of "standard" attributes. But very often you would like to add new attributes. For example you would like to keep last 50 center of mass positions of each cell to be able to plot recent cell trajectory. How would you do this? A simple approach would be to attach *e.g.* `std::queue` to the `CellG` class. This is a valid approach but it has one major disadvantage. It will require you to recompile almost entire C++ code because `CellG` class is a core class that is used by virtually every single CompuCell3D module. Also, if you would like to share the code with your colleague he would also need to recompile his or her copy of CC3D. Hence while this simple approach would certainly work it it is not the most convenient way of adding attributes. What about Python then? Yes, adding new attribute in Python is very simple:

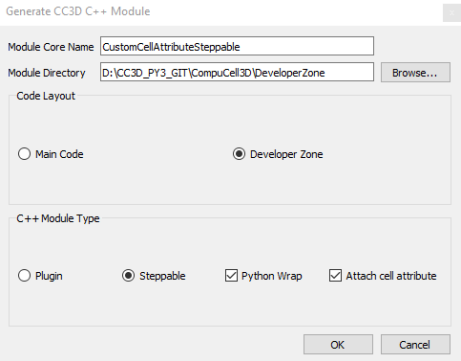
```
cell.dict['cell_x_positions'] = [0.0]*50
cell.dict['cell_y_positions'] = [0.0]*50
cell.dict['cell_z_positions'] = [0.0]*50
```

Here, we added 3 attributes each one representing last 50 positions x, y, or z coordinates of center of mass. We initialized them to be 0.0 hence the code `[0.0]*50`. In Python when you multiply list by an integer it will return a list that is contains multiple copies of the list you originally multiplied (in our case we will get a list with 50 zeros).

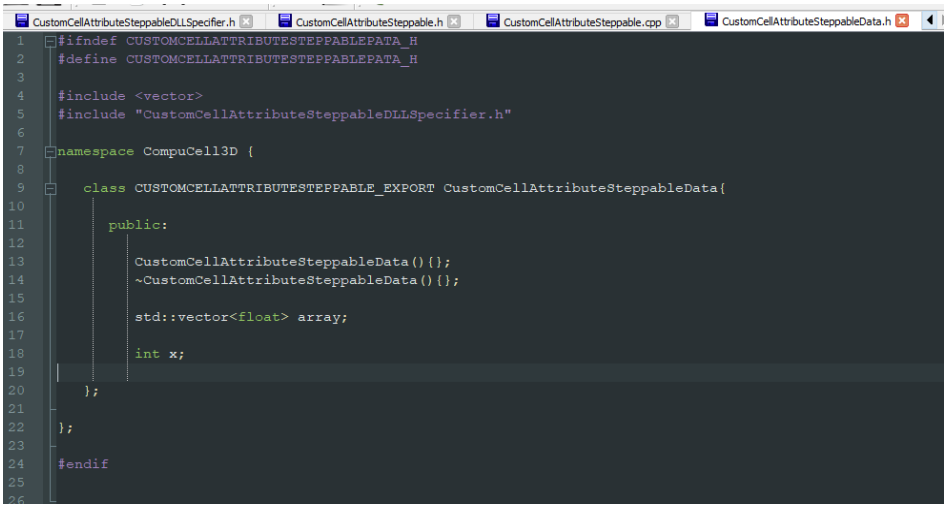
Python approach would certainly work, but what if, for efficiency reasons, you want to stay in C++ world. There is a solution for this that scales nicely i.e. it does not require recompilation of entire code and it allows to attach any C++ class as a cell attribute. This is what we will teaching you next.

20.1 Constructing Steppable with Custom Class Attached to Each Cell

We begin the usual way - open Twedit++, fo to `CC3D C++` menu and choose `Generate New Module...`` from the menu. There, as before we fill out steppable (we call it `CustomCellAttributeSteppable`) details - making sure to check `Developer Zone` radio button, but in addition to this we also check `Attach Cell Attribute` check box. This ensures that the code that Twedit++ generates contains code that will inform CC3D cell factory object to attach additional cell attribute.



We press `OK` button and the steppables code with additional attribute will get generated and the code will open in Twedit++ tabs:



The class shown in the editor window will be used during cell construction to create object of this class and attach it to each cell. In other words, once the steppable we have just created gets loaded it will tell CC3D to attach to each cell an object of class `CustomCellAttributeSteppableData`

```
#ifndef CUSTOMCELLATTRIBUTESTEPPABLEPATA_H
#define CUSTOMCELLATTRIBUTESTEPPABLEPATA_H

#include <vector>
#include "CustomCellAttributeSteppableDLLSpecifier.h"

namespace CompuCell3D {

   class CUSTOMCELLATTRIBUTESTEPPABLE_EXPORT CustomCellAttributeSteppableData{

      public:

         CustomCellAttributeSteppableData(){};
         ~CustomCellAttributeSteppableData(){};

         std::vector<float> array;

         int x;
```

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```
   };

};

#endif
```

If we look into `CustomCellAttributeSteppable` `init` function (this function is called during steppable initialization) we can see a line `potts->getCellFactoryGroupPtr()->registerClass(&customCellAttributeSteppableDataAccesso` This line is responsible for telling cell factory object that each new cell should have an object of type `CustomCellAttributeSteppableData` attached.

```
void CustomCellAttributeSteppable::init(Simulator *simulator, CC3DXMLElement *_xmlData) {

  xmlData=_xmlData;

  potts = simulator->getPotts();

  cellInventoryPtr=& potts->getCellInventory();

  sim=simulator;

  cellFieldG = (WatchableField3D<CellG *> *)potts->getCellFieldG();

  fieldDim=cellFieldG->getDim();

  ExtraMembersGroupAccessorBase *accessorPtr = &customCellAttributeSteppableDataAccessor;
  potts->getCellFactoryGroupPtr()->registerClass(accessorPtr);

  simulator->registerSteerableObject(this);

  update(_xmlData,true);

}
```

How do we know that `CustomCellAttributeSteppableData` is the class whose objects will get attached to each cell? We look into steppable header file and see the following line: `ExtraMembersGroupAccessor<CustomCellAttributeSteppableData> customCellAttributeSteppableDataAccessor;`.

This line creates special accessor object that given a pointer to a cell it will fetch attached object of type `CustomCellAttributeSteppableData`. The exact details of how this is done are beyond the scope of this manual but if you follow the pattern you will be able to attach arbitrary C++ objects to cc3d cells. The pattern is as follows:

1. Add ExtraMembersGroupAccessor member to your module - steppable or a plugin - `ExtraMembersGroupAccessor<ClassYouWantToAttach>`. In our case we add `ExtraMembersGroupAccessor<CustomCellAttributeSteppableData> customCellAttributeSteppableDataAccessor;`.

2. Add a function that accesses a pointer to this ExtraMembersGroupAccessor member - in our case we add (see code below) `ExtraMembersGroupAccessor<CustomCellAttributeSteppableData> * getCustomCellAttributeSteppableDataAccessorPtr(){return & customCellAttributeSteppableDataAccessor; }`

3. Register ExtraMembersGroupAccessor object with cell factory (we do it in the `init` function) of the steppable or plugin - see full `init` function above:

```
potts->getCellFactoryGroupPtr()->registerClass(&customCellAttributeSteppableDataAccessor);
```

```
#ifndef CUSTOMCELLATTRIBUTESTEPPABLESTEPPABLE_H
#define CUSTOMCELLATTRIBUTESTEPPABLESTEPPABLE_H
#include <CompuCell3D/CC3D.h>
#include "CustomCellAttributeSteppableData.h"
#include "CustomCellAttributeSteppableDLLSpecifier.h"

namespace CompuCell3D {

  template <class T> class Field3D;
  template <class T> class WatchableField3D;

    class Potts3D;
    class Automaton;
    class BoundaryStrategy;
    class CellInventory;
    class CellG;

  class CUSTOMCELLATTRIBUTESTEPPABLE_EXPORT CustomCellAttributeSteppable : public␣
↪Steppable {

    ExtraMembersGroupAccessor<CustomCellAttributeSteppableData>␣
↪customCellAttributeSteppableDataAccessor;

    WatchableField3D<CellG *> *cellFieldG;

    Simulator * sim;

    Potts3D *potts;

    CC3DXMLElement *xmlData;

    Automaton *automaton;

    BoundaryStrategy *boundaryStrategy;

    CellInventory * cellInventoryPtr;

    Dim3D fieldDim;

  public:

    CustomCellAttributeSteppable ();

    virtual ~CustomCellAttributeSteppable ();

    // SimObject interface

    virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);

    virtual void extraInit(Simulator *simulator);
```

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```
    ExtraMembersGroupAccessor<CustomCellAttributeSteppableData> *␣
↪getCustomCellAttributeSteppableDataAccessorPtr(){return &␣
↪customCellAttributeSteppableDataAccessor;}

    //steppable interface

    virtual void start();

    virtual void step(const unsigned int currentStep);

    virtual void finish() {}


    //SteerableObject interface

    virtual void update(CC3DXMLElement *_xmlData, bool _fullInitFlag=false);

    virtual std::string steerableName();

    virtual std::string toString();


  };

};

#endif
```

Now that we know basic rules of adding custom attributes to cells. Let's write a little bit of code that makes use use of this functionality. First we will cleanup function that parses XML (we do not need any XML parsing in our) example and then we will modify `step` function to store a product of cell `id` and current MCS in the variable `x` `CustomCellAttributeSteppableData` object (remember objects of this class will be attached to cell). We will also store x-coordinates of 5 last center of mass positions of each cell.

Here is implementation of the `update` function where we remove XML parsing code since we are not doing any XML parsing in this particular case:

```
void CustomCellAttributeSteppable::update(CC3DXMLElement *_xmlData, bool _fullInitFlag) {



    //PARSE XML IN THIS FUNCTION

    //For more information on XML parser function please see CC3D code or lookup XML␣
↪utils API

    automaton = potts->getAutomaton();

    ASSERT_OR_THROW("CELL TYPE PLUGIN WAS NOT PROPERLY INITIALIZED YET. MAKE SURE THIS␣
↪IS THE FIRST PLUGIN THAT YOU SET", automaton)
```

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```
        //boundaryStrategy has information about pixel neighbors
        boundaryStrategy = BoundaryStrategy::getInstance();

}
```

The implementation of step function is a bit more involved but not by much:

```
void CustomCellAttributeSteppable::step(const unsigned int currentStep) {

    CellInventory::cellInventoryIterator cInvItr;

    CellG * cell = 0;

    for (cInvItr = cellInventoryPtr->cellInventoryBegin(); cInvItr != cellInventoryPtr->
↪cellInventoryEnd(); ++cInvItr)

    {

        cell = cellInventoryPtr->getCell(cInvItr);

        CustomCellAttributeSteppableData * customCellAttrData =␣
↪customCellAttributeSteppableDataAccessor.get(cell->extraAttribPtr);

        //storing cell id multiplied by currentStep in "x" member of the␣
↪CustomCellAttributeSteppableData
        customCellAttrData->x = cell->id * currentStep;



        // storing last 5 xCOM positions in the "array" vector (part of ␣
↪CustomCellAttributeSteppableData)
        std::vector<float> & vec = customCellAttrData->array;
        if (vec.size() < 5) {
            vec.push_back(cell->xCOM);
        }
        else
        {
            for (int i = 0; i < 4; ++i) {
                vec[i] = vec[i + 1];
            }
            vec[vec.size() - 1] = cell->xCOM;
        }

    }

    //printouts
    for (cInvItr = cellInventoryPtr->cellInventoryBegin(); cInvItr != cellInventoryPtr->
↪cellInventoryEnd(); ++cInvItr) {
        cell = cellInventoryPtr->getCell(cInvItr);
        CustomCellAttributeSteppableData * customCellAttrData =␣
↪customCellAttributeSteppableDataAccessor.get(cell->extraAttribPtr);

```

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```
40          cerr << "cell->id=" << cell->id << " mcs = " << currentStep << " attached x␣
↪variable = " << customCellAttrData->x << endl;
41
42          cerr << "----------- up to last 5 xCOM positions ----- for cell->id " << cell->
↪id << endl;
43          for (int i = 0; i < customCellAttrData->array.size(); ++i) {
44              cerr << "x_com_pos[" << i << "]=" << customCellAttrData->array[i] << endl;
45          }
46      }
47
48  }
```

Lines 7-11 should be familiar. We iterate over all cells in the simulation and fetch a cell pointer from inventory and store it in local variable `cell`.

In line 13 we make use of out accessor object. Here we are actually fetching object of type `CustomCellAttributeSteppableData` that is attached to each cell. Note that `customCellAttributeSteppableDataAccessor.get` function takes as an input special pointer that is a member of every cell object `cell->extraAttribPtr` and returns a pointer to the object that accessor is associated with in our case it returns a pointer to `CustomCellAttributeSteppableData`.

In line 16 we assign `x` variable of the object of class `CustomCellAttributeSteppableData` to be a product of current cell `id` and current MCS.

In lines 21-33 we append current `xCOM` position of current cell to the vector `array`. We only keep last 5 positions and therefore in the `else` portion lines 25-31 we last 4 positions of the vector to the "front" of the vector and write xCOM in the last position of the vector - line 30. Note that the `else` part gets executed only if we determine that vector has already 5 elements. As you can see our attached attribute can store variable number of elements - because we append to vector. In general we can have vectors, lists, maps, queues of arbitrary objects. In fact instead of using `std::vector` it would be better to use queue because queue container makes it much easier to remove and add elements to and from the beginning and end of the container.

Warning

One thing to remember that computer has a finite memory and it you keep appending you may actually exhaust all operating system memory.

Note

Unlike in Python where we can store arbitrary objects in the list or dictionary, in C++ we need to declare which types we want to store. It makes C++ less flexible but you recoup this minor inflexibility in much faster speed of code execution

The full code for this example can be found in `CompuCell3D/DeveloperZone/Demos/CustomCellAttributesCpp` directory

20.2 Using Python scripting to modify custom C++ attributes

Sometimes you may end up in situation where in addition to modifying custom attributes in C++ you may want to modify them also in Python. In this part of the tutorial we will show you how to do it. If all we want to do is to access `x` variable from `CustomCellAttributeSteppableData` we should be "pre-wired". Well, almost. You see that when

we access objects of `CustomCellAttributeSteppableData` class from within C++ steppable where we declared the accessor object we simply type:

```
CustomCellAttributeSteppableData * customCellAttrData =␣
↪customCellAttributeSteppableDataAccessor.get(cell->extraAttribPtr)
```

However, note that `customCellAttributeSteppableDataAccessor` is declared in the "private" section of `CustomCellAttributeSteppable`. Therefore, it is not "visible" from outsides of C++ `CustomCellAttributeSteppable` class. At this point we have three potential solutions:

1. Make the accessor public - not ideal , this is a low-level object that should remain hidden

2. Make a a public function that returns a pointer to accessor - again, not ideal because then in Python or in other C++ module we would need to perform a fairly complex fetching of the `CustomCellAttributeSteppableData`

3. Declare a a public function that takes a pointer to a cell object and returns attached `CustomCellAttributeSteppableData` object. This solution seems like the cleanest of all three options

Let's modify a code and add the function that returns pointer to `CustomCellAttributeSteppableData` object. We first modify header file for the steppable class:

```
class CUSTOMCELLATTRIBUTESTEPPABLE_EXPORT CustomCellAttributeSteppable : public␣
↪Steppable {

   ExtraMembersGroupAccessor<CustomCellAttributeSteppableData>␣
↪customCellAttributeSteppableDataAccessor;

  WatchableField3D<CellG *> *cellFieldG;

  Simulator * sim;

  // ... we skipped par t fo the code here for brevity
public:

  CustomCellAttributeSteppable ();

  virtual ~CustomCellAttributeSteppable ();

  // SimObject interface

  virtual void init(Simulator *simulator, CC3DXMLElement *_xmlData=0);

  virtual void extraInit(Simulator *simulator);

   ExtraMembersGroupAccessor<CustomCellAttributeSteppableData> *␣
↪getCustomCellAttributeSteppableDataAccessorPtr(){return &␣
↪customCellAttributeSteppableDataAccessor;}

  CustomCellAttributeSteppableData * getCustomCellAttribute(CellG * cell);

  // ... we skipped par t fo the code here for brevity

  };
```

Now, we add implementation of the `getCustomCellAttribute` function to implementation file

```
CustomCellAttributeSteppableData *␣
↪CustomCellAttributeSteppable::getCustomCellAttribute(CellG * cell) {

    CustomCellAttributeSteppableData * customCellAttrData =␣
↪customCellAttributeSteppableDataAccessor.get(cell->extraAttribPtr);
    return customCellAttrData;
}
```

Note

Each time you modify header file for a C++ class that you are wrapping in Python . Make sure you also "refresh" SWIG `.i` file. It can be as simple as adding extra empty line to `CompuCell3D\DeveloperZone\pyinterface\CompuCellExtraModules\CompuCellExtraModules.i`

At this point we should be able access `CustomCellAttributeSteppableData` objects from "the outside" of the steppable class. Let us now add Python steppable where we can access `CustomCellAttributeSteppable` and `CustomCellAttributeSteppableData`:

```
1  from cc3d.core.PySteppables import *
2  from cc3d.cpp import CompuCellExtraModules
3
4
5  class CustomCellAttributePythonSteppable(SteppableBasePy):
6
7      def __init__(self, frequency=1):
8          SteppableBasePy.__init__(self, frequency)
9          self.custom_attr_steppable_cpp = None
10
11     def start(self):
12         self.custom_attr_steppable_cpp = CompuCellExtraModules.
       ↪getCustomCellAttributeSteppable()
13
14     def step(self, mcs):
15
16         print ('mcs=', mcs)
17
18         for cell in self.cell_list:
19             custom_cell_attr_data = self.custom_attr_steppable_cpp.
       ↪getCustomCellAttribute(cell)
20             print('custom_cell_attr_data=', custom_cell_attr_data)
21             print('custom_cell_attr_data.x=', custom_cell_attr_data.x)
22             custom_cell_attr_data.x = cell.id * mcs ** 2
23
24             print('after modification custom_cell_attr_data.x=', custom_cell_attr_data.x)
25             break
```

In line 12 we get access to C++ steppable object and store it in it a class variable `self.custom_attr_steppable_cpp`. In case you are wondering where `getCustomCellAttributeSteppable()` comes from, look into `CompuCell3D\DeveloperZone\pyinterface\CompuCellExtraModules\CompuCellExtraModules.i`. This SWIG wrapper file declares this function and it returns C++ steppabe object. This function is generated automatically by Twedit++:

```
%inline %{

 CustomCellAttributeSteppable * getCustomCellAttributeSteppable(){

     return (CustomCellAttributeSteppable *)Simulator::steppableManager.get(
↪"CustomCellAttributeSteppable");

   }
```

Coming back to out Python code we see that inside for loop we print to the screen the `CustomCellAttributeSteppableData` object (line `20`) and also print *x* member of this object. Later we modify and print to the screen the *x* variable of the object and we only do it for the first cell we encounter during iteration over all cells to make output more concise (see `break` statement at the end of the loop)

The output looks encouraging:

```
x_com_pos[2]=72.0625
x_com_pos[3]=72
cell->id=81 mcs = 3 attached x variable = 243
---------- up to last 5 xCOM positions ----- for cell->id 81
x_com_pos[0]=79
x_com_pos[1]=78.8936
x_com_pos[2]=78.8
x_com_pos[3]=78.7273
mcs= 3
custom_cell_attr_data= <cc3d.cpp.CompuCellExtraModules.CustomCellAttributeSteppableData; proxy of <Swig Object of type 'CompuCell3D::CustomCellAttributeSteppableData *' at 0x000001CCAED37330> >
custom_cell_attr_data.x= 3
after modification custom_cell_attr_data.x= 9
CALLING CLOSE EVENT FROM  SIMTAB
EXITING WITH ERROR CODE= 0

Process finished with exit code 0
```

We can see - look at the lines:

```
custom_cell_attr_data.x= 3
after modification custom_cell_attr_data.x= 9
```

that we can access and modify *x* variable of the `CustomCellAttributeSteppableData` object that is attached to each cell.

What about the `array` member of `CustomCellAttributeSteppableData`. Remember, in C++ it is of type `std::vector<float>`. Can we access it? Can we modify it? Let's us try:

```
1  from cc3d.core.PySteppables import *
2  from cc3d.cpp import CompuCellExtraModules
3
4
5  class CustomCellAttributePythonSteppable(SteppableBasePy):
6
7      def __init__(self, frequency=1):
8          SteppableBasePy.__init__(self, frequency)
9          self.custom_attr_steppable_cpp = None
10
11     def start(self):
12         self.custom_attr_steppable_cpp = CompuCellExtraModules.
   ↪getCustomCellAttributeSteppable()
13
14     def step(self, mcs):
15         print('mcs=', mcs)
16
```

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```
17          for cell in self.cell_list:
18              custom_cell_attr_data = self.custom_attr_steppable_cpp.
↪getCustomCellAttribute(cell)
19              print('custom_cell_attr_data=', custom_cell_attr_data)
20              print('custom_cell_attr_data.x=', custom_cell_attr_data.x)
21
22              custom_cell_attr_data.x = cell.id * mcs ** 2
23
24              print('after modification custom_cell_attr_data.x=', custom_cell_attr_data.x)
25
26              print('custom_cell_attr_data.array=', custom_cell_attr_data.array)
27              print('custom_cell_attr_data.array[0]=', custom_cell_attr_data.array[0])
28
29              if len(custom_cell_attr_data.array) < 5:
30                  custom_cell_attr_data.array.push_back(100.0)
31              print('custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] = ',
32                  custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1])
33
34              break
```

In lines 26-27 we print the type of `custom_cell_attr_data.array` as well as the first element. Later, in lines 29-32 we are appending elements to the vector using `push_back` C++ function (because `array` is a C++ object wrapped in Python). Notice that we are doing double append for first cell. First append (`push_back`) happens in C++ and in Python we are doing a second one. This , somewhat artificial example shows how to access and modify custom attributes from C++ and from Python in a single simulation.

Here is the output:

```
---------- up to last 5 xCOM positions ----- for cell->id 81
x_com_pos[0]=78.8936
x_com_pos[1]=78.8936
x_com_pos[2]=78.7333
x_com_pos[3]=78.3404
mcs= 3
custom_cell_attr_data= <cc3d.cpp.CompuCellExtraModules.CustomCellAttributeSteppableData; proxy of <Swig Object of type 'CompuCell3D::CustomCellAttributeSteppableData *' at 0x00000196312DF090> >
custom_cell_attr_data.x= 3
after modification custom_cell_attr_data.x= 9
custom_cell_attr_data.array= <cc3d.cpp.PlayerPython.vectorfloat; proxy of <Swig Object of type 'std::vector< float,std::allocator< float > > *' at 0x00000196312DF0F0> >
custom_cell_attr_data.array[0]= 100.0
custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] =  22.934782028198242
CALLING CLOSE EVENT FROM  SIMTAB
EXITING WITH ERROR CODE= 0

Process finished with exit code 0
```

20.2.1 Adding a complex type to attached attribute and accessing it from Python

So far things worked as a charm. We were able to access simple type variables (x), STL vectors `array`. So, perhaps we can try adding something more complex to the `CustomCellAttributeSteppableData`, for example let us add `std::map<long int, std::vector<int> >` which is C++ dictionary (map) that uses long integers as keys and stores vectors of type integer:

```
#ifndef CUSTOMCELLATTRIBUTESTEPPABLEPATA_H
#define CUSTOMCELLATTRIBUTESTEPPABLEPATA_H

#include <vector>
#include "CustomCellAttributeSteppableDLLSpecifier.h"

namespace CompuCell3D {
```

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```
   class CUSTOMCELLATTRIBUTESTEPPABLE_EXPORT CustomCellAttributeSteppableData{

      public:

         CustomCellAttributeSteppableData(){};
         ~CustomCellAttributeSteppableData(){};

         std::vector<float> array;
         std::map<long int, std::vector<int> > simple_map;

         int x;

   };

};

#endif
```

After we recompile (remember to refresh `CompuCellExtraModules.i`) and try running the following Python code:

```
from cc3d.core.PySteppables import *
from cc3d.cpp import CompuCellExtraModules


class CustomCellAttributePythonSteppable(SteppableBasePy):

    def __init__(self, frequency=1):
        SteppableBasePy.__init__(self, frequency)
        self.custom_attr_steppable_cpp = None

    def start(self):
        self.custom_attr_steppable_cpp = CompuCellExtraModules.
↪getCustomCellAttributeSteppable()

    def step(self, mcs):
        print('mcs=', mcs)

        for cell in self.cell_list:
            custom_cell_attr_data = self.custom_attr_steppable_cpp.
↪getCustomCellAttribute(cell)
            print('custom_cell_attr_data=', custom_cell_attr_data)
            print('custom_cell_attr_data.x=', custom_cell_attr_data.x)

            custom_cell_attr_data.x = cell.id * mcs ** 2

            print('after modification custom_cell_attr_data.x=', custom_cell_attr_data.x)

            print('custom_cell_attr_data.array=', custom_cell_attr_data.array)
            print('custom_cell_attr_data.array[0]=', custom_cell_attr_data.array[0])

            if len(custom_cell_attr_data.array) < 5:
                custom_cell_attr_data.array.push_back(100.0)
```

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```
            print('custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] = ',
                custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1])

            simple_map = custom_cell_attr_data.simple_map

            print('simple_map.size()=', simple_map.size())
```

we will get an error when we try to get number of elements stored in the map (should be 0):

```
Traceback (most recent call last):
  File "D:\CC3D_PY3_GIT\cc3d\CompuCellSetup\sim_runner.py", line 77, in run_cc3d_project
    exec(code, globals(), locals())
  File "D:\CC3D_PY3_GIT\CompuCell3D\DeveloperZone\Demos\CustomCellAttributesPython\
↪Simulation\CustomCellAttributesPython.py", line 6, in <module>
    CompuCellSetup.run()
  File "D:\CC3D_PY3_GIT\cc3d\CompuCellSetup\simulation_setup.py", line 117, in run
    main_loop_fcn(simulator, simthread=simthread, steppable_registry=steppable_registry)
  File "D:\CC3D_PY3_GIT\cc3d\CompuCellSetup\simulation_setup.py", line 583, in main_loop_
↪player
    steppable_registry.step(cur_step)
  File "D:\CC3D_PY3_GIT\cc3d\core\SteppableRegistry.py", line 169, in step
    steppable.step(_mcs)
  File "D:\CC3D_PY3_GIT\CompuCell3D\DeveloperZone\Demos\CustomCellAttributesPython\
↪Simulation\CustomCellAttributesPythonModules.py", line 36, in step
    print('simple_map.size()=', simple_map.size())
AttributeError: 'SwigPyObject' object has no attribute 'size'
```

Why the error? Simply put we did not tell SWIG about the complex types we are using for member `simple_map`. You may ask how come before when we had `std::vector<int> array;` things worked. They worked because elsewhere in the CompuCell3D main python wrapper we told SWIG about template `std::vector<int>`. However now that we are dealing with `std::map<long int, std::vector<int> > simple_map;` we need to tell SWIG how to make those object available. It is actually quite easy to do. We add the following lines to `CompuCellExtraModules.i`:

```
%template (vector_int) std::vector<int>;
%template (map_long_vector_int)std::map<long int, std::vector<int> >;
```

For each template we are using in the our extra attribute we give it a name (e.g. `vector_int`) and list its type - `%template (vector_int) std::vector<int>;`

After this fix when we try to run the earlier Python code we would get the following output:

```
mcs= 0
custom_cell_attr_data= <cc3d.cpp.CompuCellExtraModules.CustomCellAttributeSteppableData; proxy of <Swig Object of type 'CompuCell3D::CustomCellAttributeSteppableData *' at 0x0000026A3506F720> >
custom_cell_attr_data.x= 0
after modification custom_cell_attr_data.x= 0
custom_cell_attr_data.array= <cc3d.cpp.PlayerPython.vectorfloat; proxy of <Swig Object of type 'std::vector< float,std::allocator< float > > *' at 0x0000026A3506F750> >
custom_cell_attr_data.array[0]= 23.0
custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] =  100.0
simple_map.size()= 0
```

As we can see the size of the map comes up as zero because we did not put any elements in it. Let's add a code that puts something in the map:

```
from cc3d.core.PySteppables import *
from cc3d.cpp import CompuCellExtraModules

```

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```
4
5  class CustomCellAttributePythonSteppable(SteppableBasePy):
6
7      def __init__(self, frequency=1):
8          SteppableBasePy.__init__(self, frequency)
9          self.custom_attr_steppable_cpp = None
10
11     def start(self):
12         self.custom_attr_steppable_cpp = CompuCellExtraModules.
   ↪getCustomCellAttributeSteppable()
13
14     def step(self, mcs):
15         print('mcs=', mcs)
16
17         for cell in self.cell_list:
18             custom_cell_attr_data = self.custom_attr_steppable_cpp.
   ↪getCustomCellAttribute(cell)
19             print('custom_cell_attr_data=', custom_cell_attr_data)
20             print('custom_cell_attr_data.x=', custom_cell_attr_data.x)
21
22             custom_cell_attr_data.x = cell.id * mcs ** 2
23
24             print('after modification custom_cell_attr_data.x=', custom_cell_attr_data.x)
25
26             print('custom_cell_attr_data.array=', custom_cell_attr_data.array)
27             print('custom_cell_attr_data.array[0]=', custom_cell_attr_data.array[0])
28
29             if len(custom_cell_attr_data.array) < 5:
30                 custom_cell_attr_data.array.push_back(100.0)
31             print('custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] = ',
32                   custom_cell_attr_data.array[len(custom_cell_attr_data.array) - 1])
33
34             simple_map = custom_cell_attr_data.simple_map
35
36             print('simple_map.size()=', simple_map.size())
37             vec = CompuCellExtraModules.vector_int()
38             vec.push_back(20)
39             vec.push_back(30)
40             simple_map[cell.id] = vec
41
42             print('simple_map[cell.id]=', simple_map[cell.id])
43
44             break
```

In line 37 we create a C++ vector of integers using `` CompuCellExtraModules.vector_int()`` call. Remember, `vector_int` is precisely template identifier we added in SWIG `CompuCellExtraModules.i` file. Now we are simply invoking constructor for this type. In the next two lines `38-39` we push back two integers to the newly created vector and finally in line `40` we store this vector in the map that is part fo the object that is attached to a cell. To check if we can retrieve the stored vector we use code from line `42`. The output is as follows:

```
mcs= 1
custom_cell_attr_data= <cc3d.cpp.CompuCellExtraModules.CustomCellAttributeSteppableData; proxy of <Swig Object of type 'CompuCell3D::CustomCellAttributeSteppableData *' at 0x0000026A35D044B0> >
custom_cell_attr_data.x= 1
after modification custom_cell_attr_data.x= 1
custom_cell_attr_data.array= <cc3d.cpp.PlayerPython.vectorfloat; proxy of <Swig Object of type 'std::vector< float,std::allocator< float > > *' at 0x0000026A35D04540> >
custom_cell_attr_data.array[0]= 22.9375
custom_cell_attr_data.array[len(custom_cell_attr_data.array)-1] =  100.0
simple_map.size()= 1
simple_map[cell.id]= (20, 30)
```

20.3 Summary

In this section we learned how to attache C++ attribute to each cell, how to modify it from C++ and how to interact with complex types that are part of the attached attribute at the Python level.

CHAPTER

TWENTYONE

DEBUGGING CC3D USING GDB

Sometimes when you execute simulation and encounter software crash it is useful to do a quick introspection to see what went wrong. IN this section we will show you how to inspect CC3D call trace using GDB.

Note

Provided recipe works only on OSX and Linux

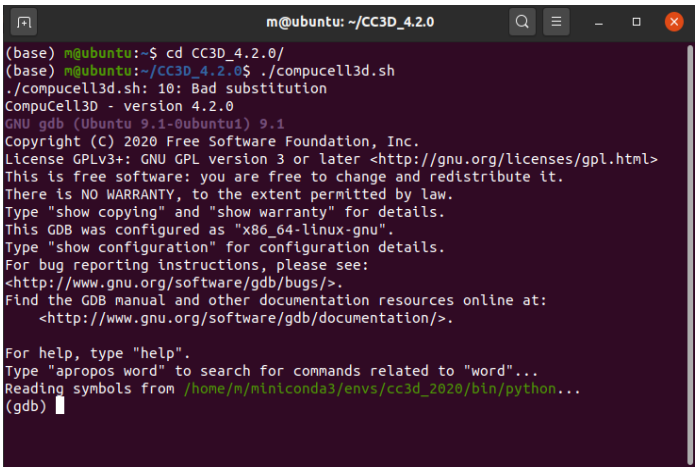
First it is useful to create a copy of CC3D run scripts because we will be modifying those. This way you will have a copy to revert to after you are done with debugging. LEt us start with modifications to `compucell3d.sh` (on OSX `compucell3d.command`) script. This script launches Player and allows you to run simulation. When we open `compucell3d.sh` in editor, towards the end of the file you will see a line that looks as follows:

```
${PYTHON_EXEC} ${PREFIX_CC3D}/lib/site-packages/cc3d/player5/compucell3d.pyw $* --
↪currentDir=${current_directory}
```

we will replace this line with

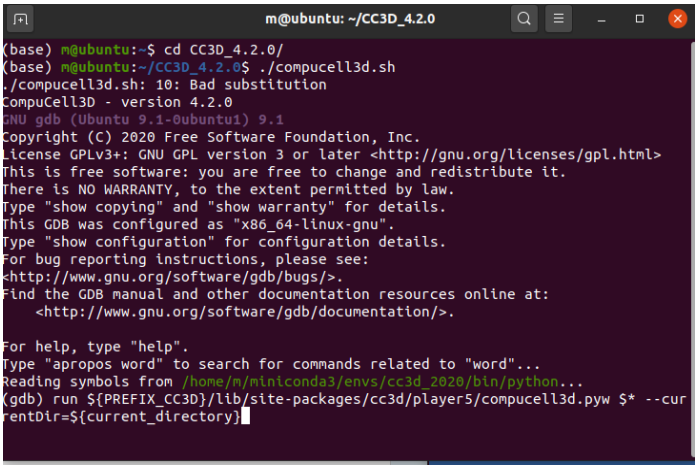
```
gdb ${PYTHON_EXEC}
```

Save the script and run it. As a result we will be dropped to gdb shell that is setup to debug Python scripts (`${PYTHON_EXEC}` points to Python interpreter)



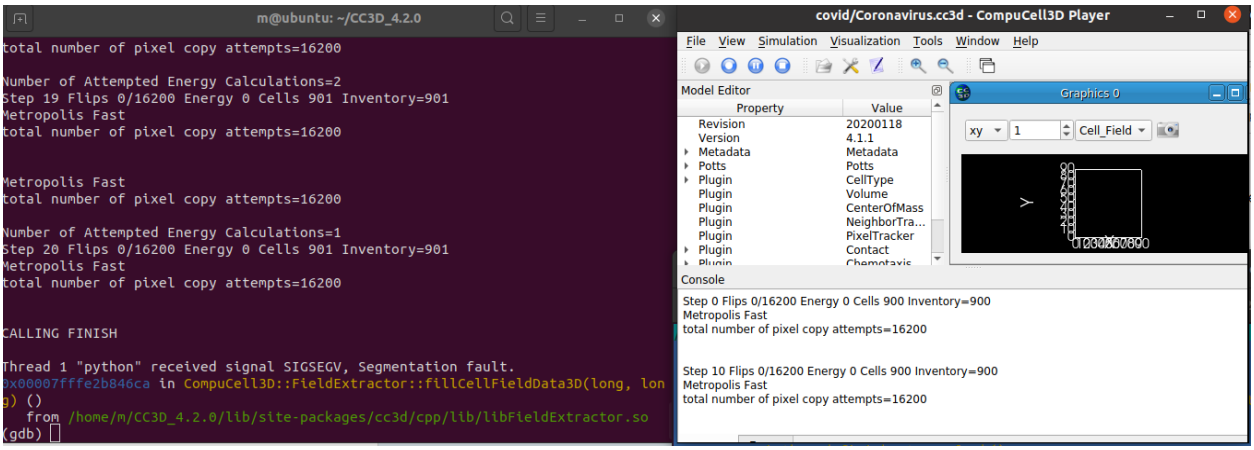
Next, in Python shell we will run actual player by typing

```
run ${PREFIX_CC3D}/lib/site-packages/cc3d/player5/compucell3d.pyw $* --currentDir=$
↪{current_directory}
```



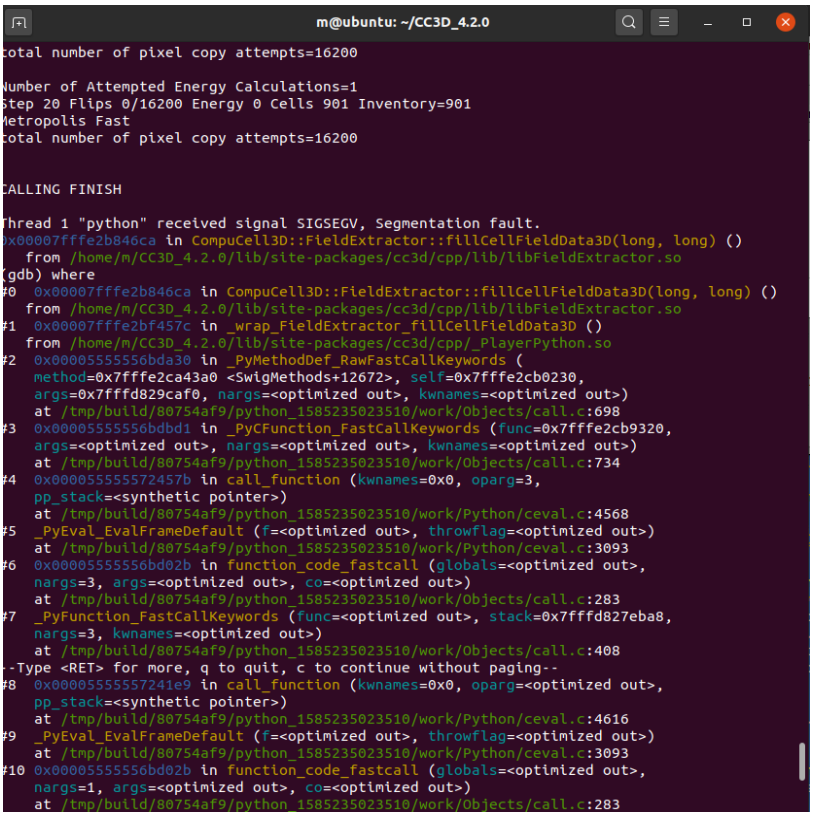
the `run` command tells gdb to start running the program that we passes to gdb when we invoked gdb shell. In out case this program is a Python interpreter, exactly what we want. The remaining arguments of the `run` line are the arguments we are passing to the program we are debugging. In our case we pass `${PREFIX_CC3D}/lib/site-packages/cc3d/player5/compucell3d.pyw $* --currentDir=${current_directory}` which means that Python interpreter will run `player5/compucell3d.pyw` executable script that takes `$* --currentDir=${current_directory}` as arguments

After the payer pops up we load simulation and run it as if it were a normal CC3D run. This time however we are running in the debubugger shell an as you can see in the left panel we are getting debug output. In this case we see a crash occurring:



The crash happened at the end of the simulation (we turned off thread synchronization code to trigger crash)

As you can see, the crash happened in `fillCellFieldData3D` function. To get full call stack trace we can type `where` in the gdb shell to get more information



When you experience CC3D crash it is useful to take this extra step and get more information to figure out where the actual problem occurs. Sending this information to developers can fast-track the software patch

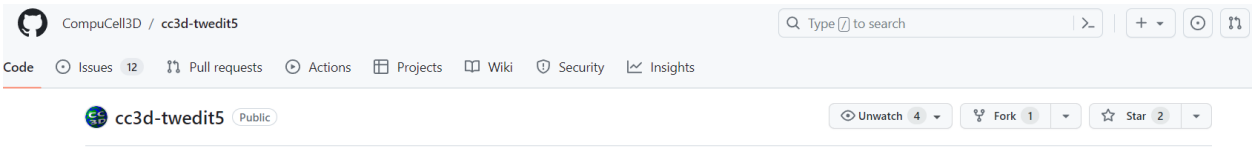
CHAPTER

TWENTYTWO

GETTING STARTED WITH CC3D GUI CODE

Working on the GUI code for CC3D requires some knowledge about PyQt5, access to a decent Python IDE (e.g. PyCharm) and a bit of setup. In this section we will show you how to get started working on either Player of Twedit++ code.

First thing you will need to do is to fork Player or Twedit repository. To do that, log in to your github.com account and fork e.g. Twedit code - https://github.com/CompuCell3D/cc3d-twedit5.:



Once you forked the code, go ahead and clone it from your repository (not from CompuCell3D repository).

To clone repository you follow command pattern below:

```
cd d:\src\
git clone git@github.com:<your_github_name>/cc3d-twedit5.git
```

or if you want to clone Player

```
cd d:\src\
git clone git@github.com:<your_github_name>/cc3d-player5.git
```

The reason it is important that you first fork repository to your own account instead of cloning it directly from CompuC3ll3D account is that if you for you will be able to push changes to the forked version of Player or Twedit++ whereas if you cloned directly from our repository you will not be able to store your code edits on the github server.

22.1 Installing IDE

While there are many IDEs we recommend PyCharm Community Edition. This is an excellent Python tool that you can use free of charge. Please google the download link for for this software and install it on your machine. Make sure to use community Edition, not the professional one if you do not want to pay for the software

22.2 Running CompuCell3D User interface code in PyCharm

Warning

The following instructions are for Windows. If you are on OSX or Linux there should not be much of a difference except that when you copy directories you may us soft links and the layout of the Python environment is slightly different on OSX/Linux than it is on Windows. We will point out the differences later in the text.

As you may know by now, CompuCell3D is distributed in the form of conda packages. Typically, you would use a binary installer that under the hood installs distribution of Miniconda, then installs mamba (python package manager that os much faster than conda package manager) and then uses mamba to install CompuCell3D. Now, as a developer you will need to do those steps manually. First, let's install conda - here is tha link and installation instructions:

https://docs.conda.io/projects/miniconda/en/latest/index.html

Once you install the latest version of Miniconda for your operating system you should install mamba into `base` conda environment:

```
conda install -c conda-forge mamba
```

Note, `-c conda-forge` points to `conda-forge` channel that is one of the most reliable repositories of conda packages.

Once mamba is installed you should create new conda environment for the latest version of CC3D. As of this writing, this version is 4.4.1.3. Hence we do the following:

```
conda create -n cc3d_4413_310 python=3.10
```

Next, we activate this environment:

```
conda activate cc3d_4413_310
```

and install latest version of CompuCell3D:

```
mamba install -c conda-forge -c compucell3d compucell3d=4.4.1
```

It may take few minutes for all packages to download. Notice, we are now sourcing our packages from two conda package repositories: `conda-forge` and `compucell3d`.

Once CompuCell3d is installed, verify that you can run Player:

```
python -m cc3d.player5
```

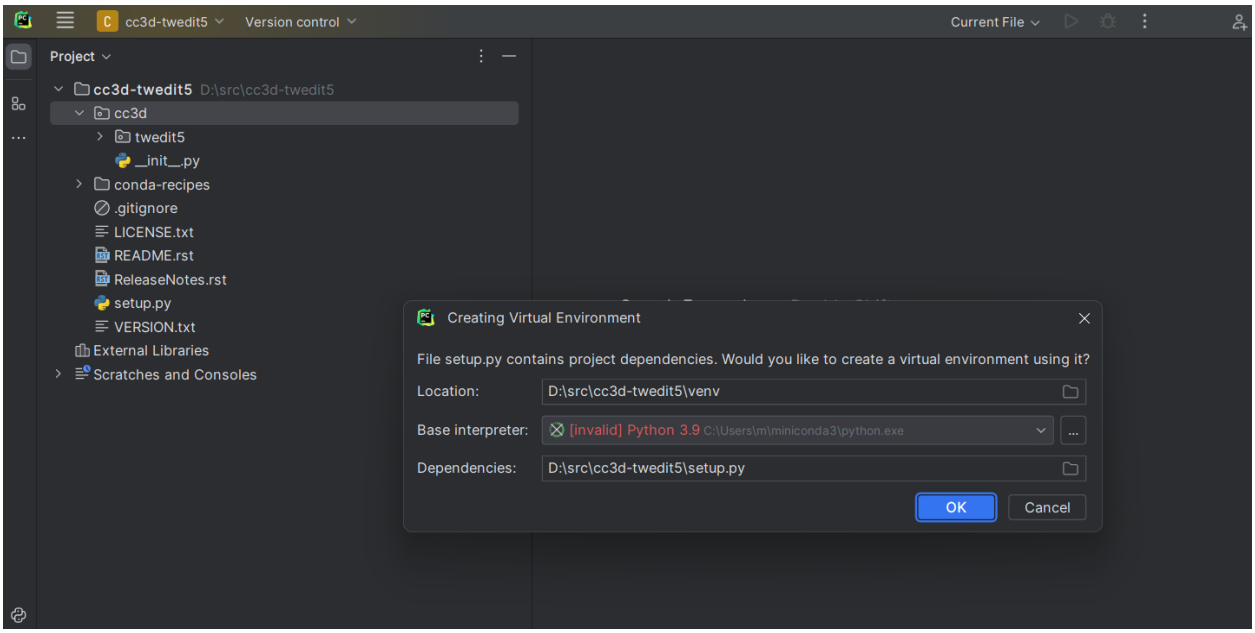
If this command works and the Player UI opens, try running one of the demo simulations to make sure everything works and if there are no errors, we should be ready for the next step - configuring your IDE so that you can run either Player or Twedit++ from PyCharm

22.3 Configuring IDE to run Twedit++

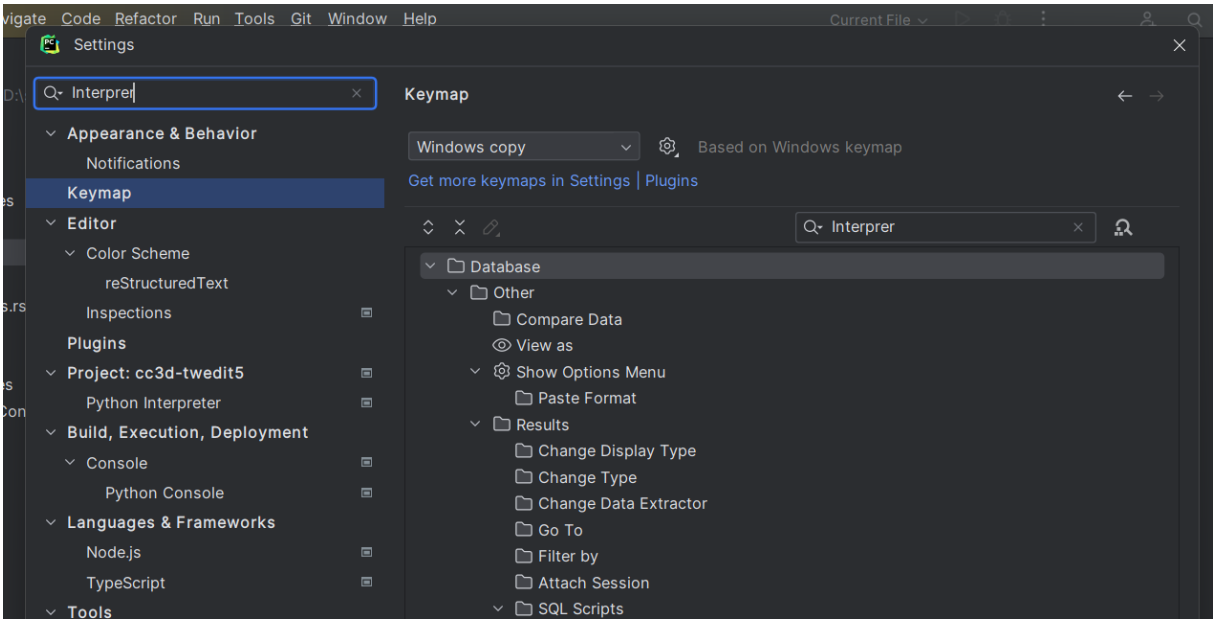
Even though we will show how to run Twedit++ using PyCharm, the steps for Player ara analogous.

First thing we need to do is to open cc3d-twedit5 repository in PyCharm:

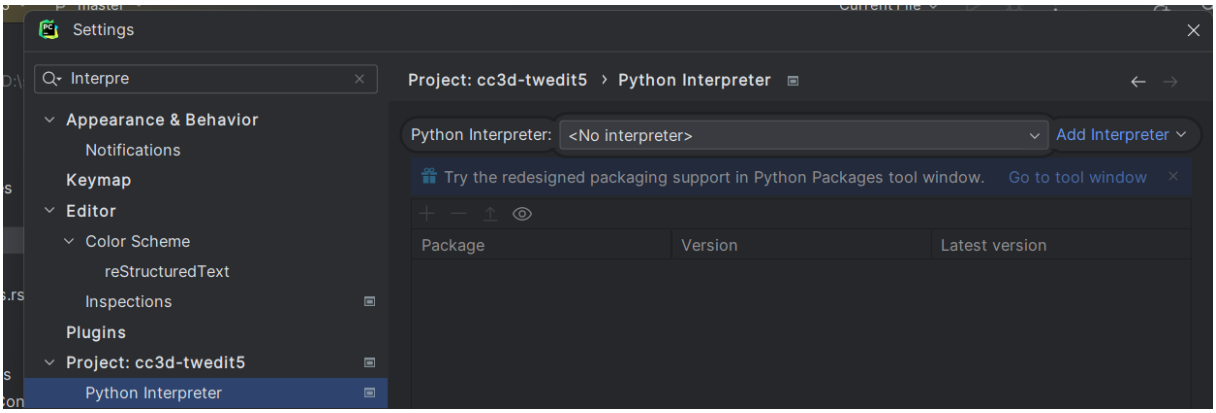
If you see a prompt (dialog) to setup Python interpreter, choose **Cancel**



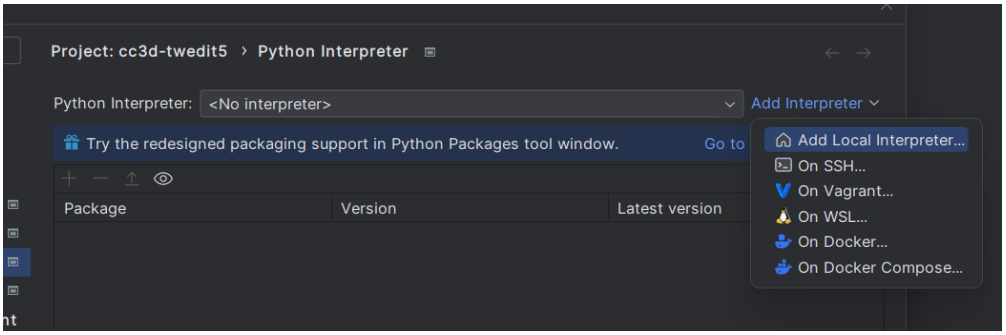
We will use different configuration dialog to configure Python Interpreter for cc3d-twedit5. Simply, got to File->Settings and the following configuration dialog will open up:



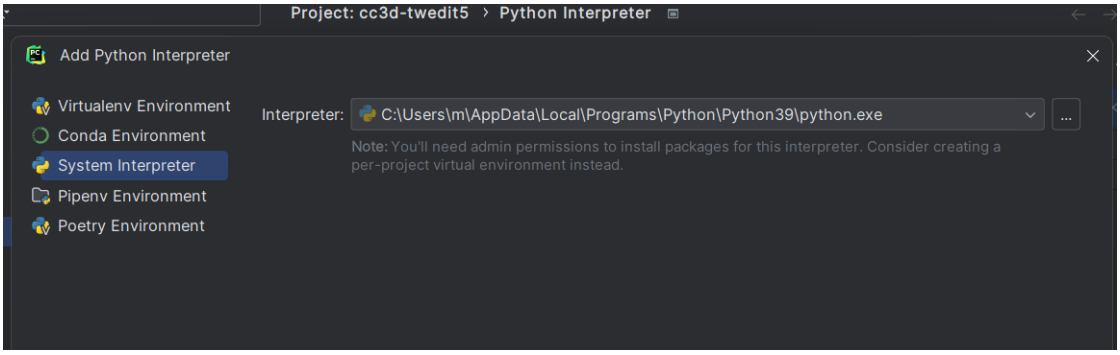
Type interpreter in the search bar above and click Python Interpreter option from the left panel of the popup dialog:



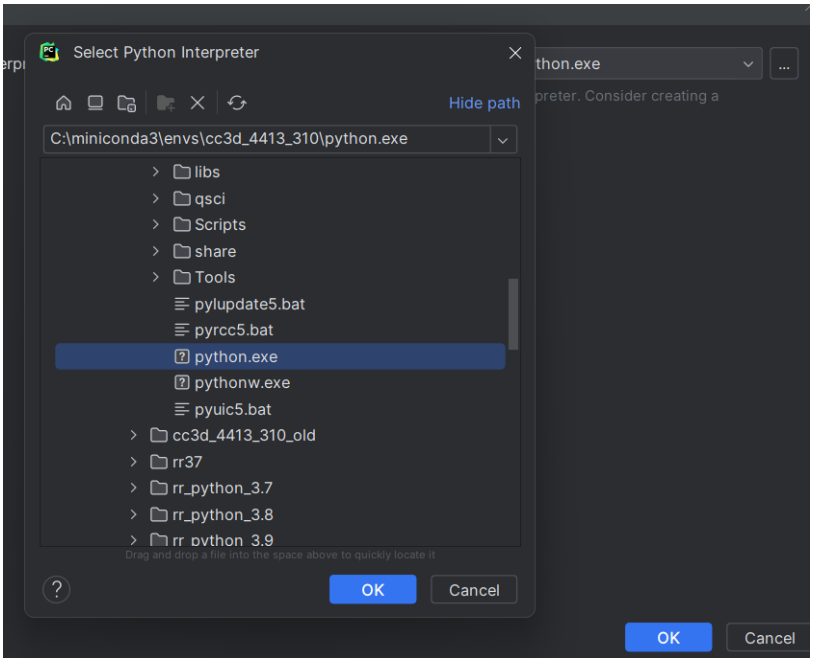
Click Add Interpreter (top right blue button on the dialog), choose “Add Local Interrpreter”



Choose “System Interpreter”



and navigate to the place where your newly created conda environment is):



In my case it was installed to `c:\miniconda3\envs\cc3d_4413_310\python.exe`

After this Click OK on all open dialogs and your newly-created interpreter will be added to the list of Python interpreters available to PyCharm

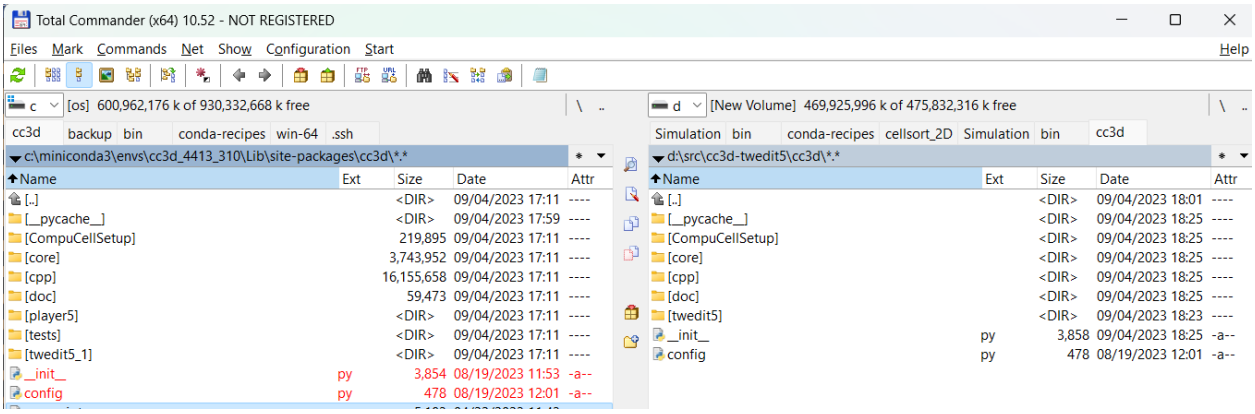
22.3.1 Finalizing the setup

To finalize the setup you need to do few other things:

1. Copy `__init__.py` and `config.py` from `c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d`

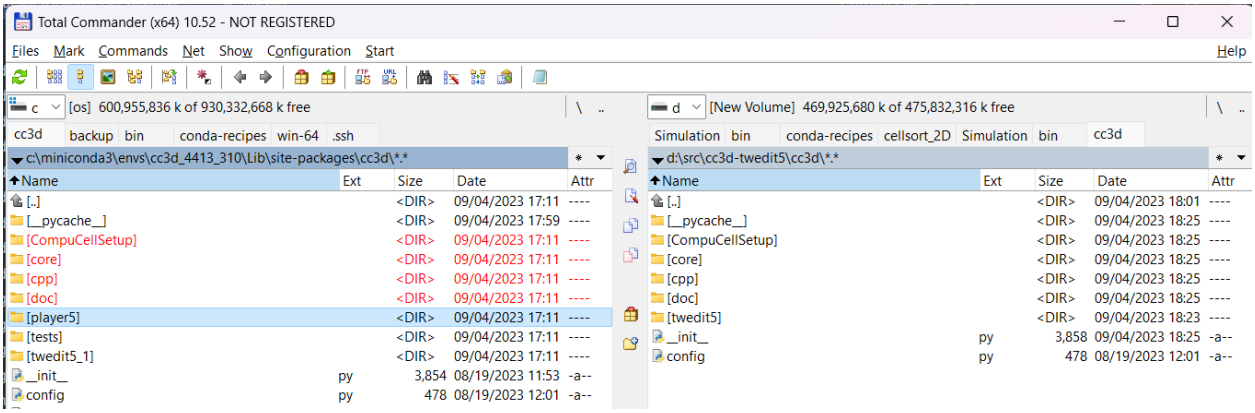
> **Note**
>
> If you are on OSX or Linux your cc3d package will be located in `/Users/m/miniconda3/envs/cc3d_4412_310/lib/python3.10/site-packages/cc3d`.

to `cc3d` folder inside the folder into which you cloned your cc3d-twedit5 repository:



Comment out line 76 and 77 in `__init__.py`

Copy the following directories: `CompuCellSetup`, `core`, `cpp`, `doc` from `c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d` to `cc3d` folder inside the folder into which you cloned your cc3d-twedit5 repository:



Note

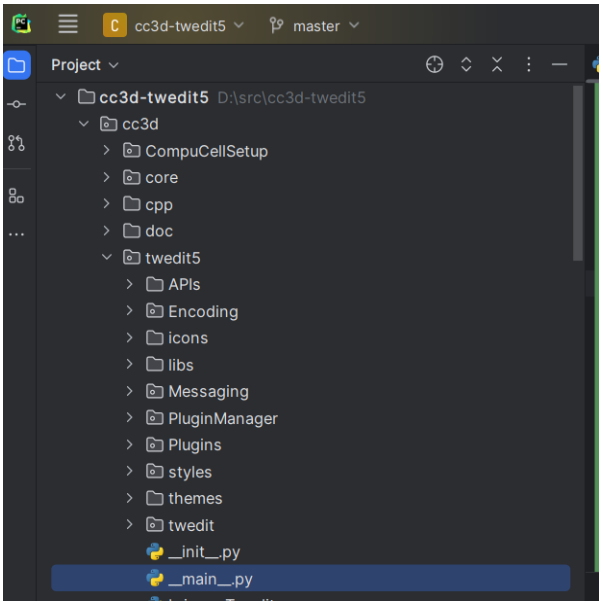
If you are on OSX or Linux instead of copying directories you may make soft-links from those directories in the conda environment to appropriate destination within your cloned repo folder

Finally, rename `c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d\twedit5` to `c:\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d\twedit5_1`.

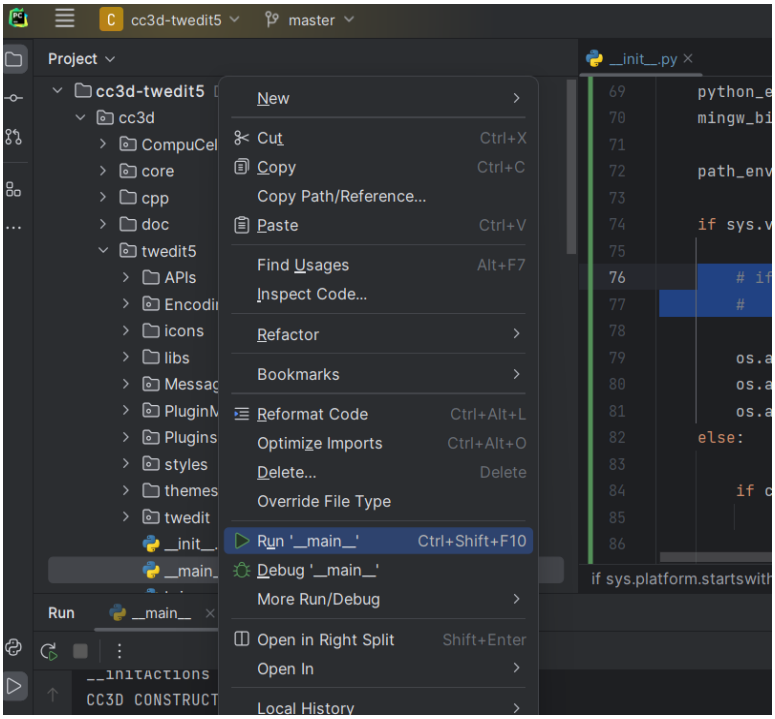
This last step is to make sure that when you run twedit5 from PyCharm it will be the code from your repository that is run, and not the code that got installed with CompuCell3D.

Now you should run the Twedit++ (cc3d.twedit5) from your PyCharm:

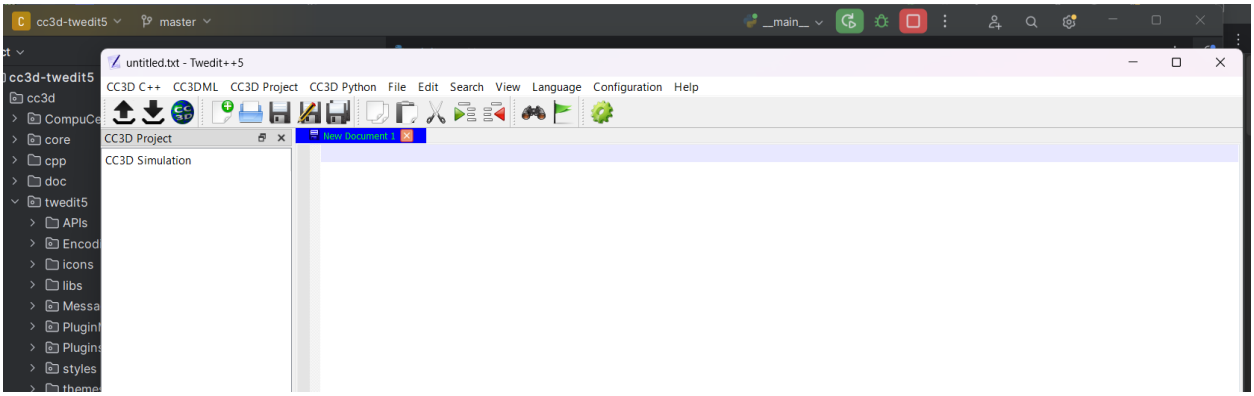
In the left panel of PyCharm "unfold" folders until you reach `cc3d-twedit5\cc3d\twedit5\__main__.py`



Right-click on this file and choose, “Run” (or “Debug” if you want to start debugging session - somthing we will cover next):



Twedit++ should open up:



At this point you are ready to do UI development using PyCharm

22.4 Making Changes

Your local Player repository and your Miniconda version of Player can either remain two separate directories, or you can soft-link the files you would change. We focus on Windows here since it requires a small workaround.

On Windows, you can copy over the changes each time you need to test Player. If you edited files in the `Configuration` directory, for instance, run this command to test that. Be careful about where you copy to. It may be wise to create a backup of your Miniconda CC3D Player directory if you are not sure.

Other commands besides `cp` should work, too, like `robocopy` or `rsync` if you prefer.

How to Edit .ui (PyQt) Files:

1. First, install Qt Designer.
2. Next, open the `.ui` file you want to edit from the command line. Adjust the path as necessary. `designer C:\Users\Me\cc3d\player5\Configuration\cc3D_prefs.ui`
3. Nearly every PyQt component we use is inside of a layout. If you can't move something right away, select it or its parent component and use the 'Break Layout ' button. When you have things roughly well-positioned, select everything that lacks a layout and assign it one (usually either Horizontal Layout or Vertical Layout) to align the components.
4. After you saving your changes, you should use the following command to translate the `.ui` file into a `.py` file. Since these Python files need to be auto-generated each time we make changes in Designer, you should never edit them manually. Note that we use a `cp` command before the `pyuic` command if we're on Windows since the local repository and Miniconda files need to be synched. Again, adjust the directory name if you are editing something outside of `player5\Configuration`.

```
cp -fr C:\Users\Me\cc3d\cc3d-player5\cc3d\player5\Configuration\* C:\ProgramData\
↪miniconda3\envs\name-of-your-environment\Lib\site-packages\cc3d\player5\Configuration\␣
↪&& pyuic5 c:\ProgramData\miniconda3\envs\cc3d_4413_310\Lib\site-packages\cc3d\player5\
↪Configuration\cc3D_prefs.ui -o c:\ProgramData\miniconda3\envs\cc3d_4413_310\Lib\site-
↪packages\cc3d\player5\Configuration\ui_configurationdlg.py
```

Finally, view your changes with `python -m cc3d.player5`. Commit and push both the `.ui` and `.py` files to the Player5 repos.

CHAPTER

TWENTYTHREE

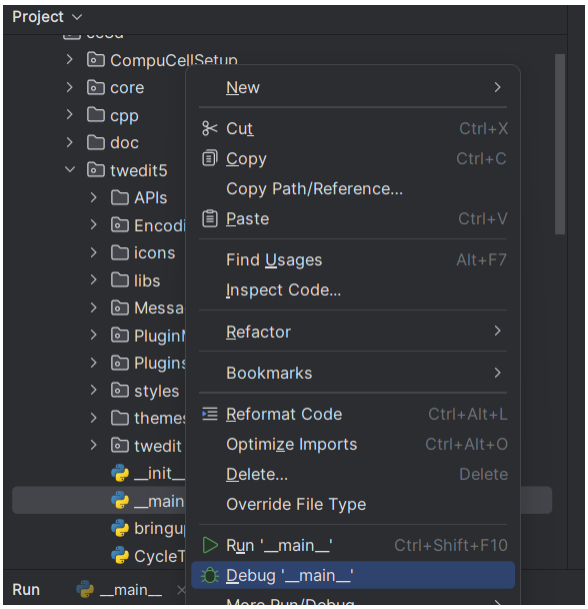
DEBUGGING UI IN PYCHARM

Once you set your PyCharm to launch Twedit++ or Player (see instructions in *Running Player and Twedit++ from PyCharm*) it is a good time to ask a question why go through all this trouble? The answer is - debuggin capabilities. Sure you can use `pdb` but it is not terribly efficient. PyCharm offers great debugging capabilities and in this section we will explore how to do do debugging in PyCharm. We will work with Twedit++ code but the same principles apply to Player , or for that matter to any other Python project.

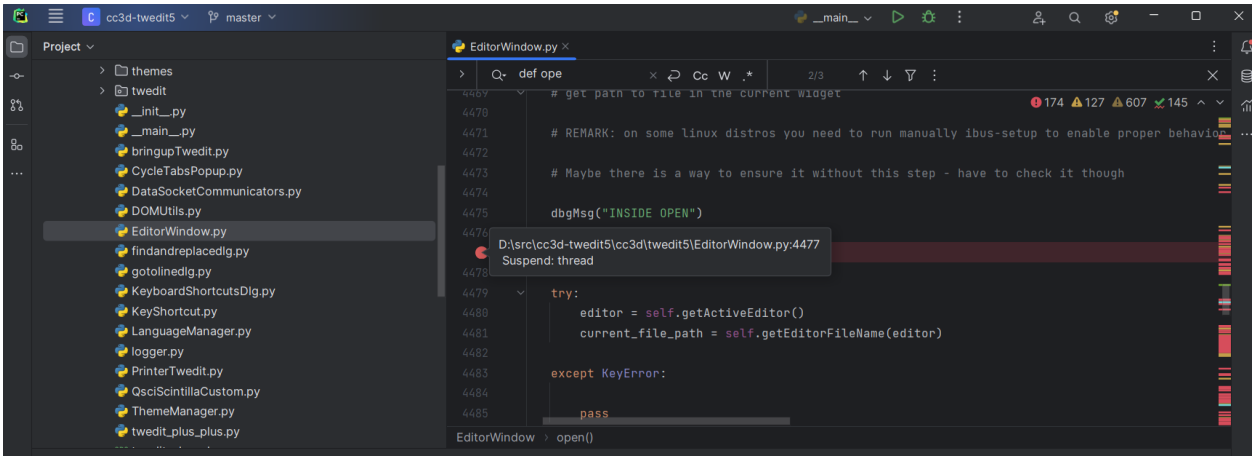
You may want to look at the PyCharm documentation that teaches you about capabilities of the PyCharm debugger. https://www.jetbrains.com/help/pycharm/debugging-your-first-python-application.html#where-is-the-problem

This section complements this tutorial and shows you how the debugging session may look like when working with Player or Twedit++.

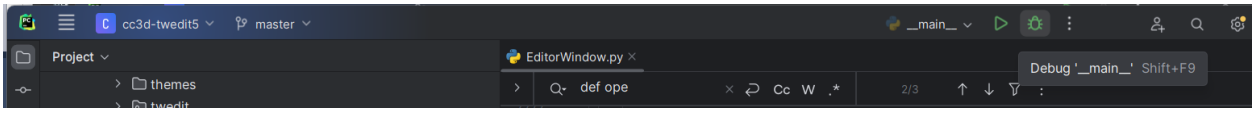
Let us begin but instead of choosing `Run` option after right-clicking on `__main__.py` click `Debug`



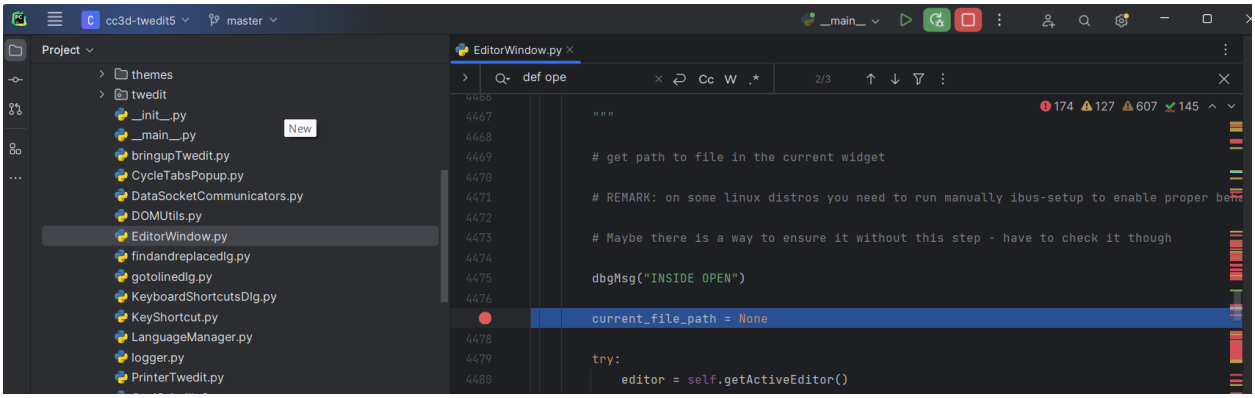
now you are running the code in the debug mode. Not terribly interesting. So let's put a breakpoint inside `EditorWindow.py` (click on the margin where the code lines are displayed). Let's go inside the function `open(self)`



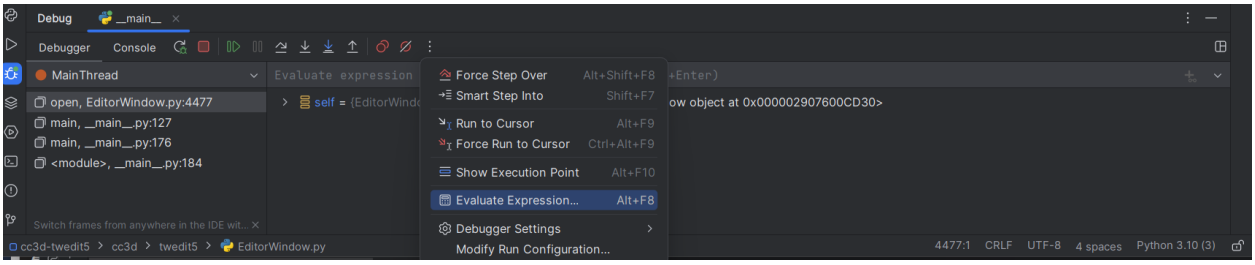
hit `Debug` from the toolbar



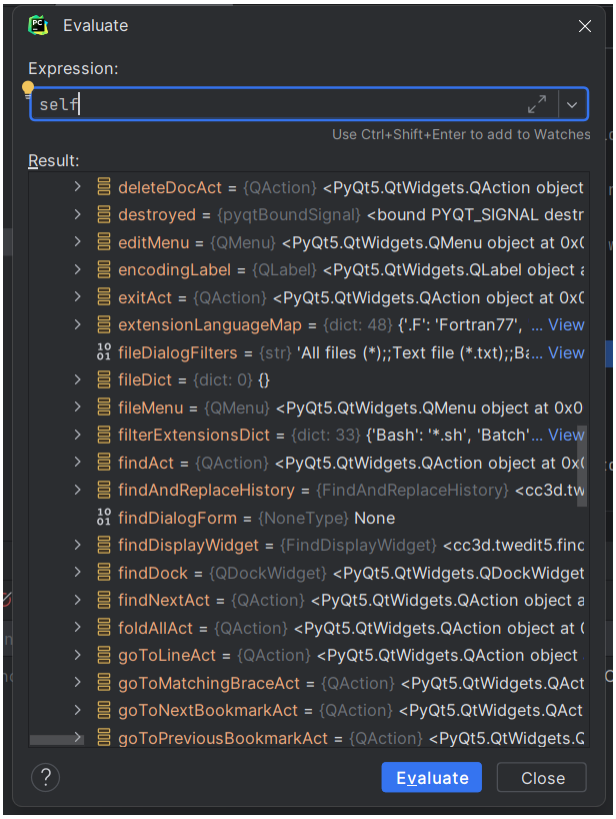
Nothing will happen but when you try opening a document (`File->Open`) The cursor code execution will stop at the line at which you put a breakpoint. You may need to manually switch window focus so that PyCharm is on top.



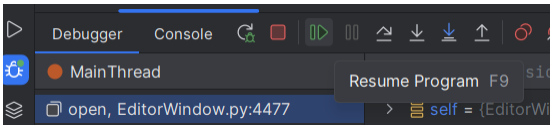
Click three dots and open `Evaluate Expression..` (or hit `Alt-F8`)



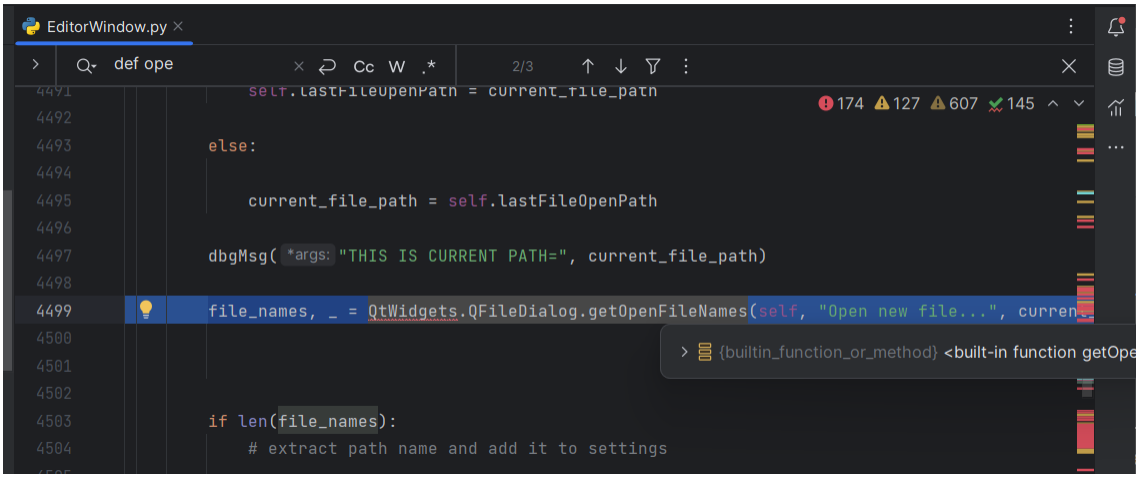
end in the top line of the popup window type `self`, hit `Enter` and scroll down to see what members class `EditorWindow` has:



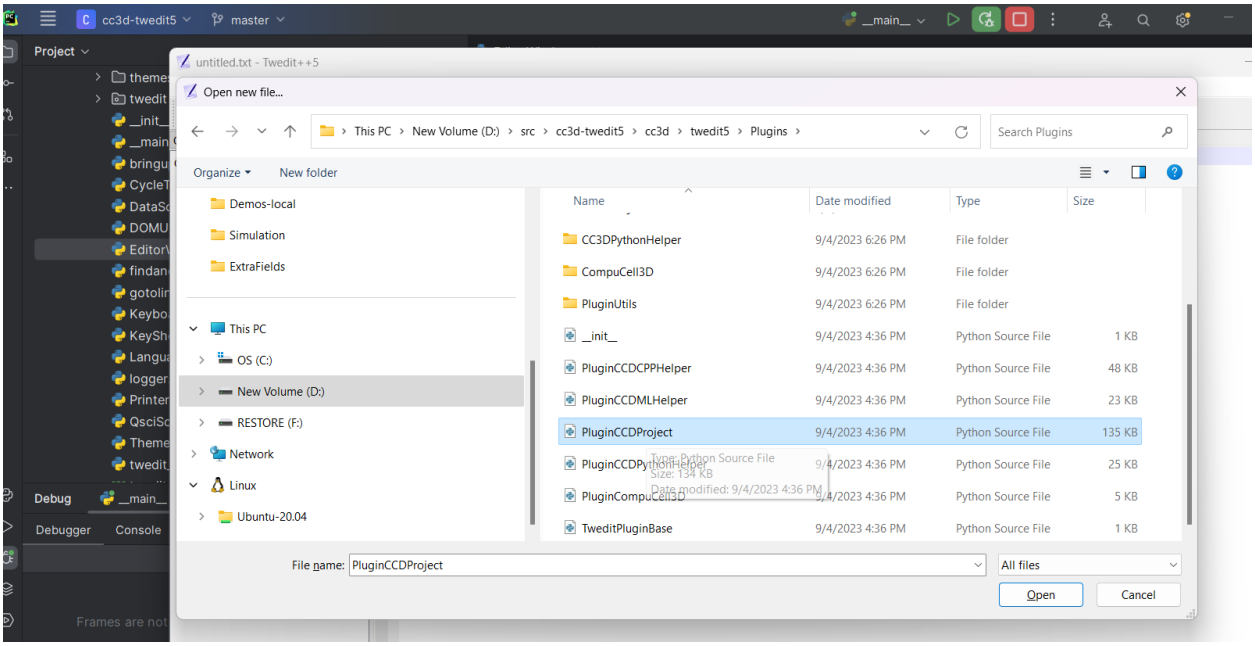
Take a look at the `fileDict` member of `EditorWindow` class. It is empty now. so lets complete opening a document - to do that you need to move past the breakpoint. There are two ways: you can either click `Resume` button (or click `F9`)



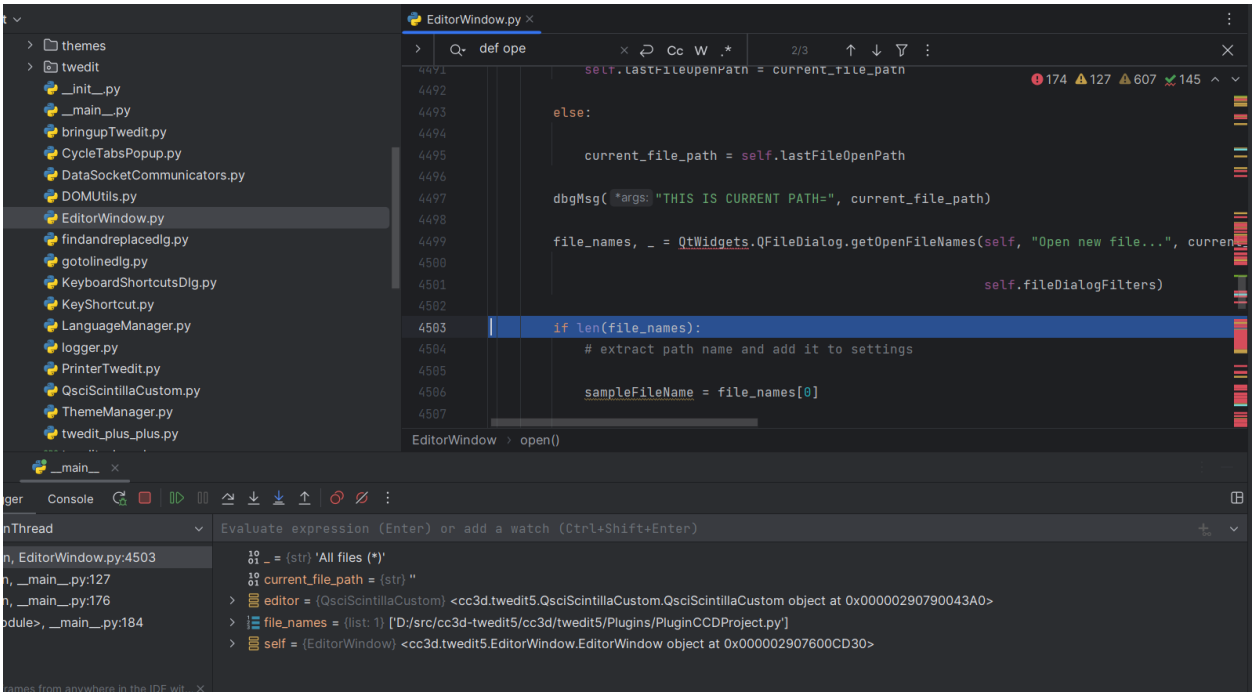
or you can keep clicking `F8` and step through the code line by line. The second option might be useful when you want to see what really the code is doing. Let's keep clicking `F8` until we get to the line that starts with `file_names, _ = QtWidgets.QFileDialog.getOpenFileNames`



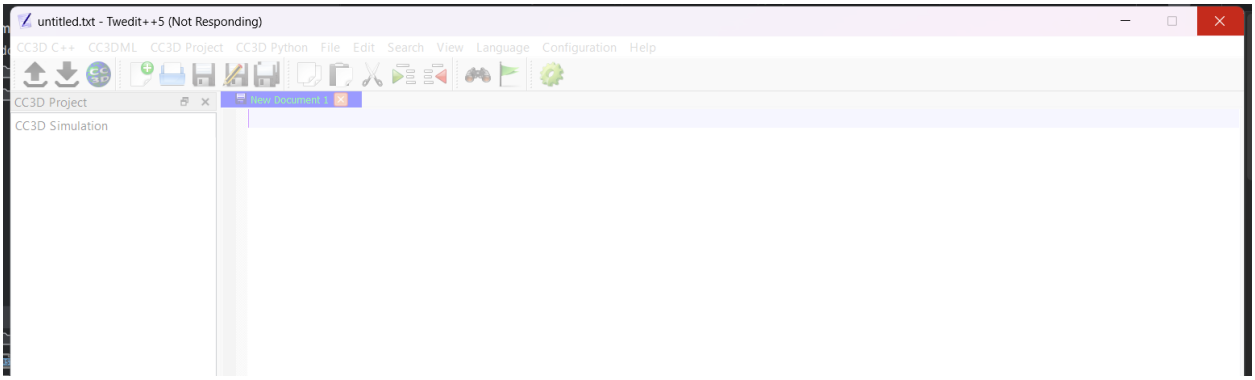
After we get through the line that we are parked now the `File Open` dialog will display and we can select a Python file



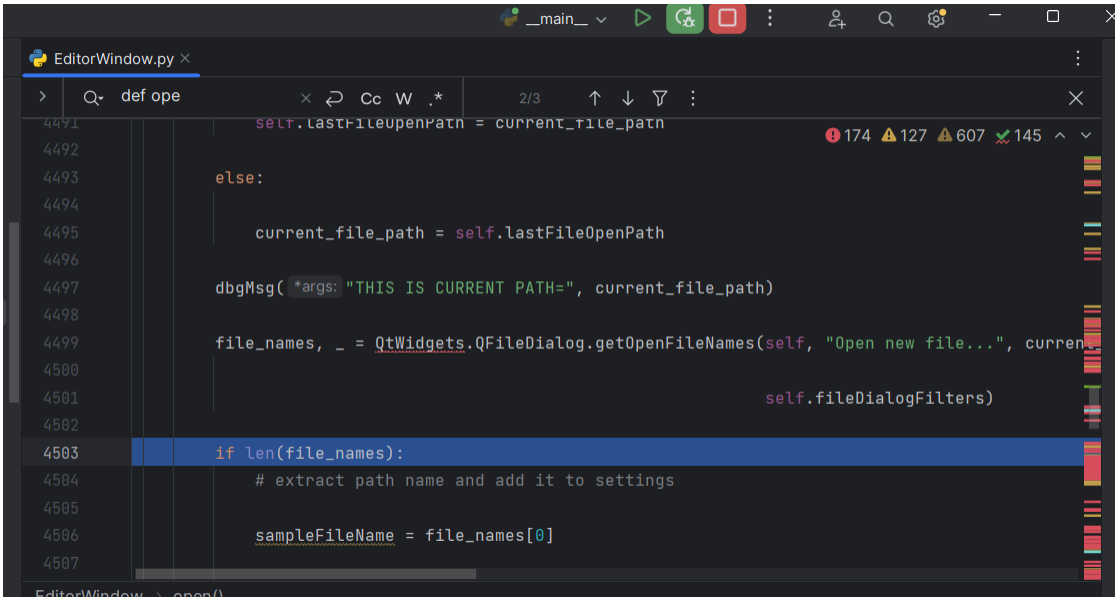
If we and if we click Open on the `File Open` dialog we will be brought back to the code



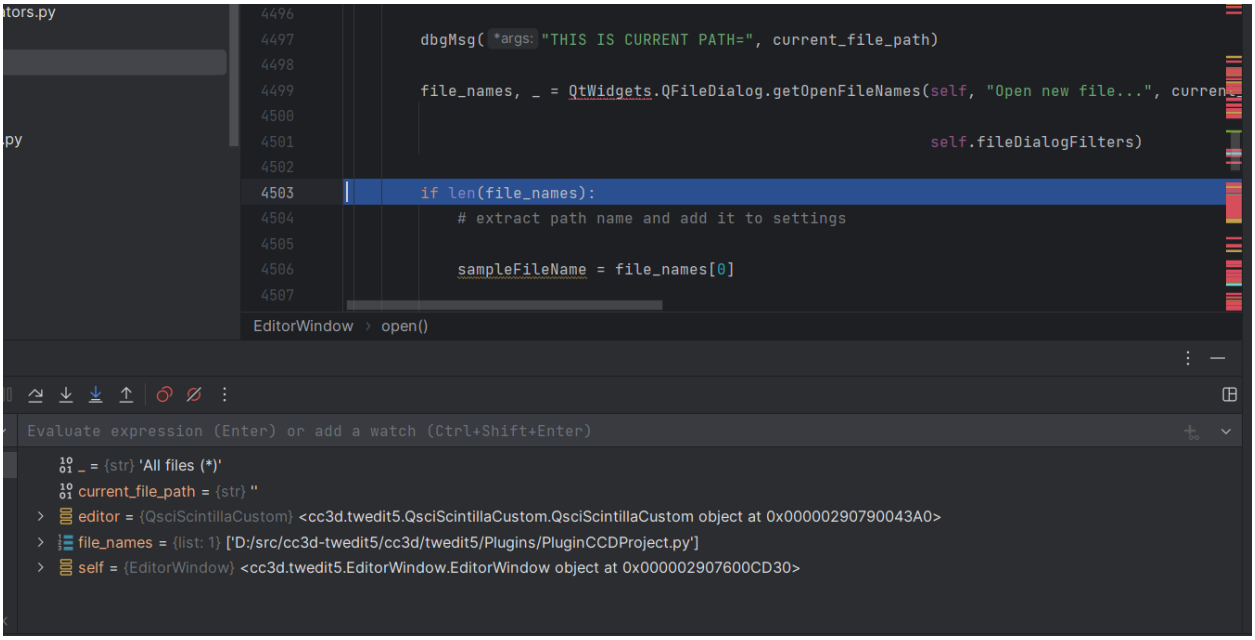
We are past the line that opened a dialog, and where we completed file selection. Interestingly, no text appeared in the editor yet.



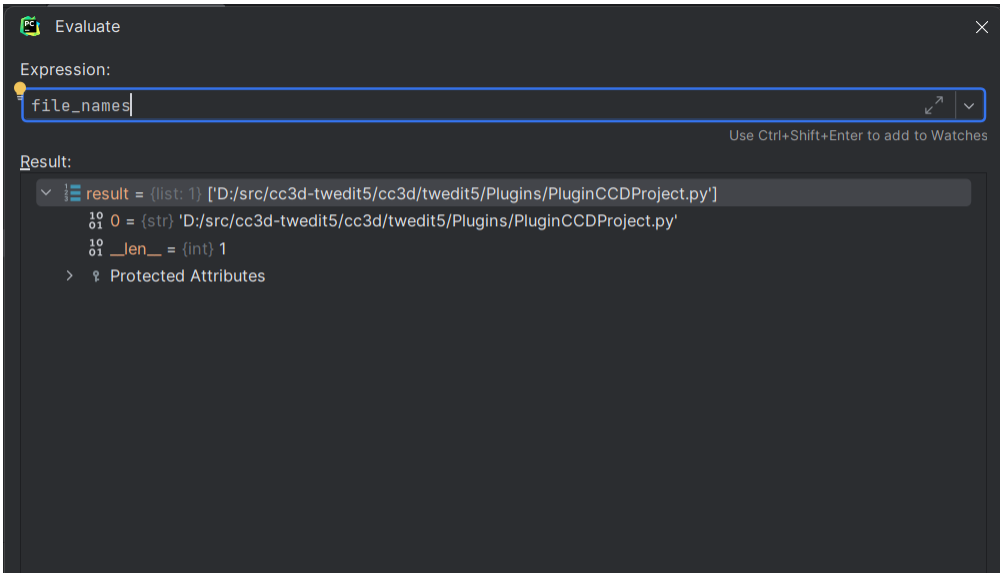
This is not a coincidence. We are in the middle of the process (method) that opens a file in the editor. So far we have completed file selection process but we have not yet "displayed" the content of the file in Twedit++. Let's see where we are in the code:



We are just past the `File Open` dialog line and we already selected the file. Notice that the bottom panel displays variable `file_names` that contains the list of files selected in a `File Open` dialog (it was just one file)

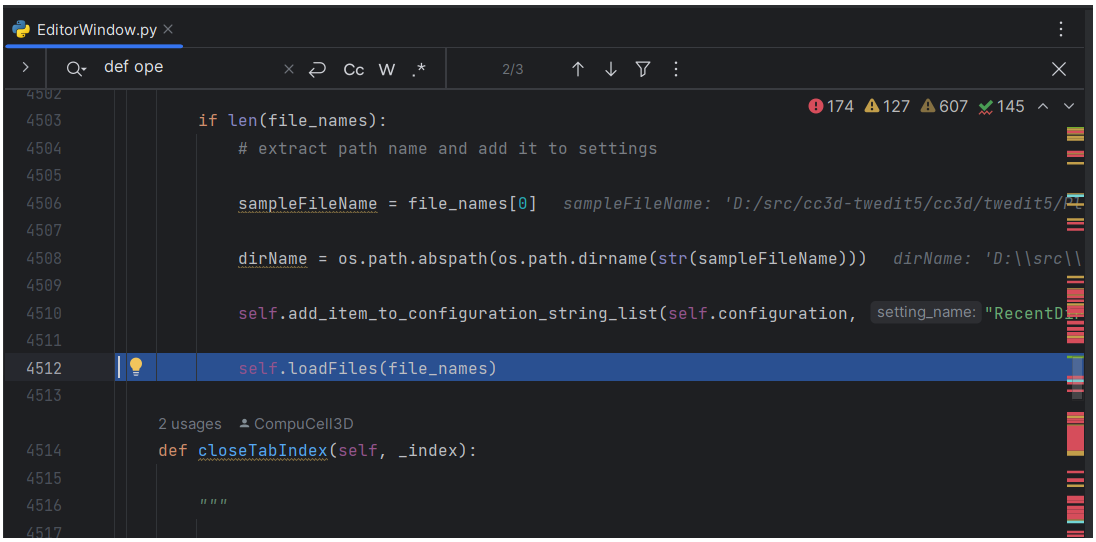


We can either exlpore the values in the bottom panel or we can use `Evaluate Expression` window - the results will be the same and it is a matter of preference which method of "code exploration" you choose:

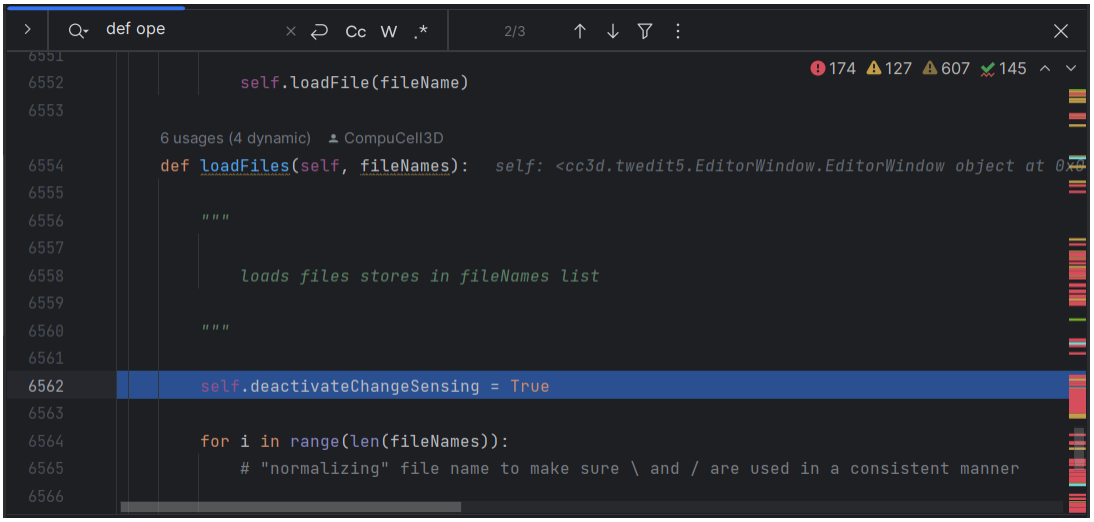


So far we have learned how to step-through "live" code and inspect application state (values of variables).

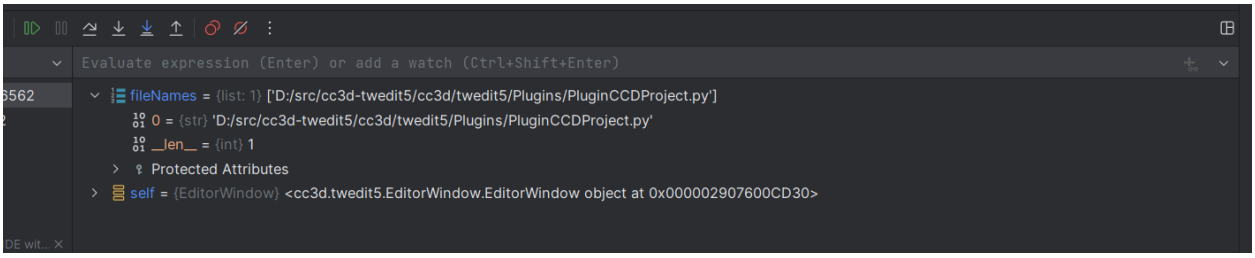
Let's continue clicking `F8` until we hit the line with `self.loadFiles`



If we hit `F8` again (do not do it yet) the actual files we selected will be loaded and their content will be displayed. Instead let's hit `F7`. `F7` will step-into the function `loadFiles` and we will be able to inspect what is going on there:



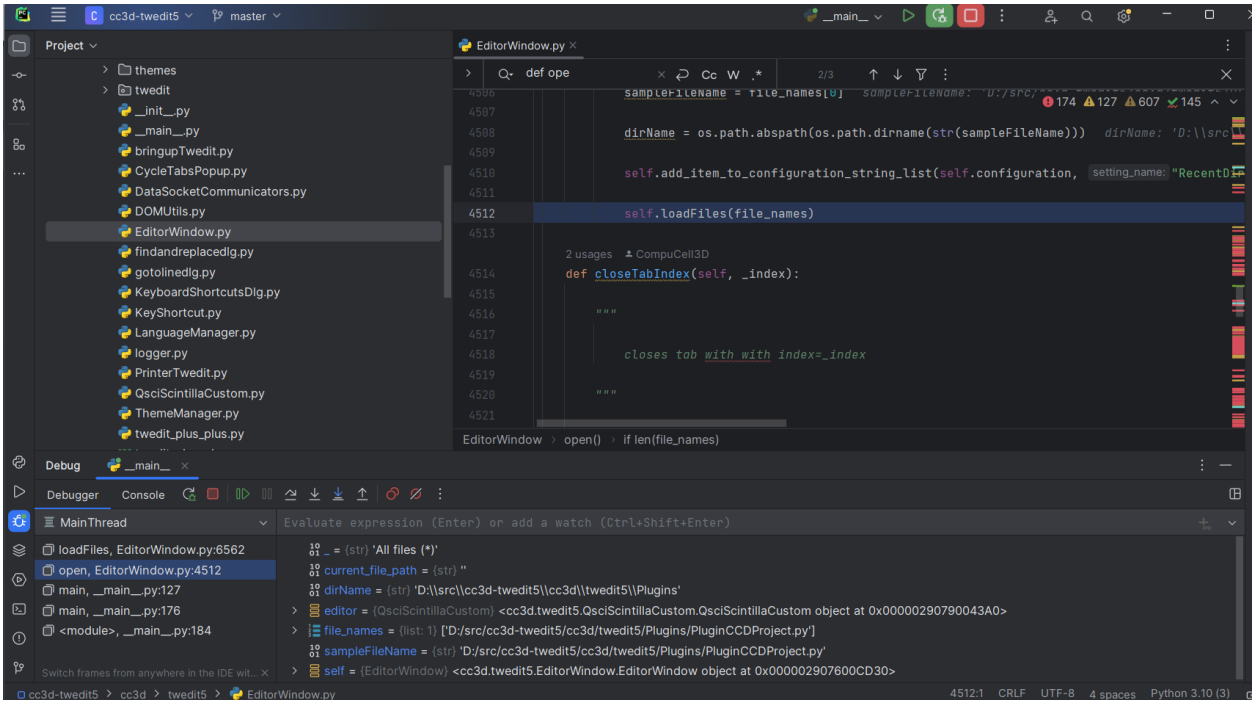
For example if we look at the bottom panel we see that the `file_names` were passed from function `open` to function `loadFiles` and it is now referred to as `fileNames`



Before we step through `loadFiles` function let's explore the call stack management panel (the left panel):

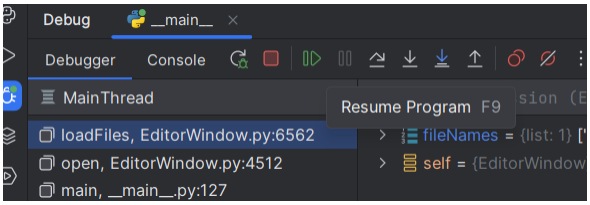
Note that the line that is highlighted - it says `loadFiles, EditorWindow.py` which means that we are inside function `loadFiles` that is part of the `EditorWindow.py` module. A line belo says `open,EditorWindow.py` which means that we got to function `loadFiles` from function `open` .

Let's click the line that says `open,EditorWindow.py`.

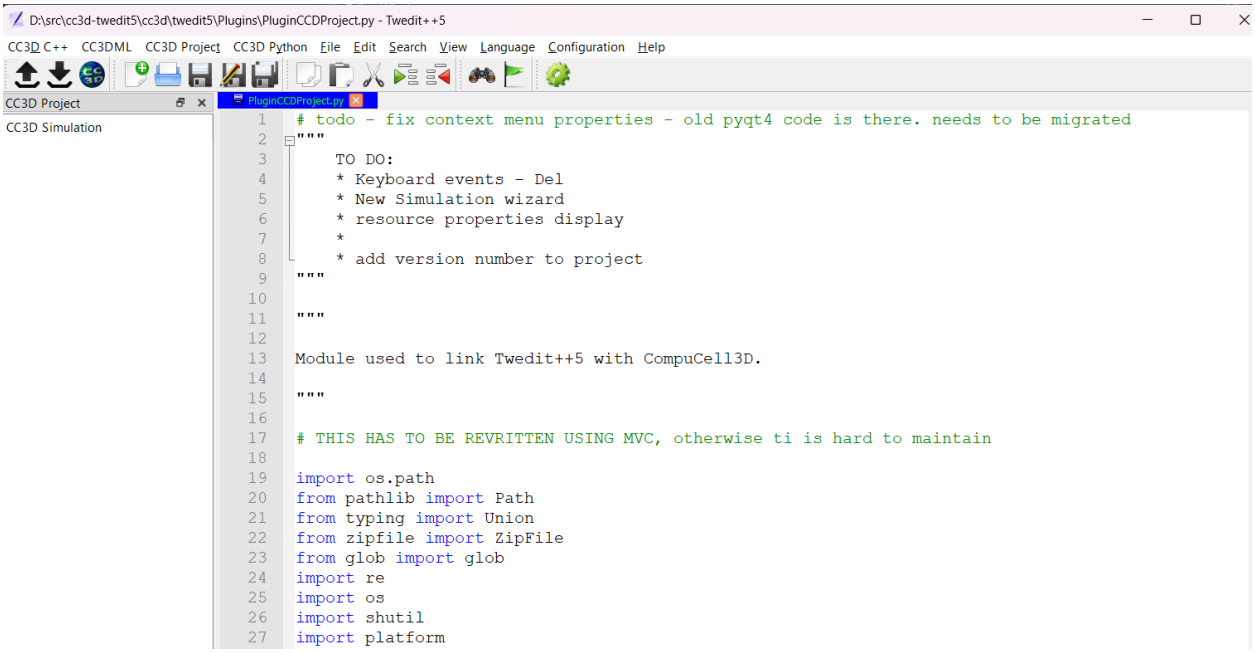


and notice that brings us back to the place from where we clicked `F7`. In general you can leverage Call Stack panel and move up and down the call stack, and at each step you can use `Evaluate Expression` (`Alt-F8`) window to inspect the state of your app.

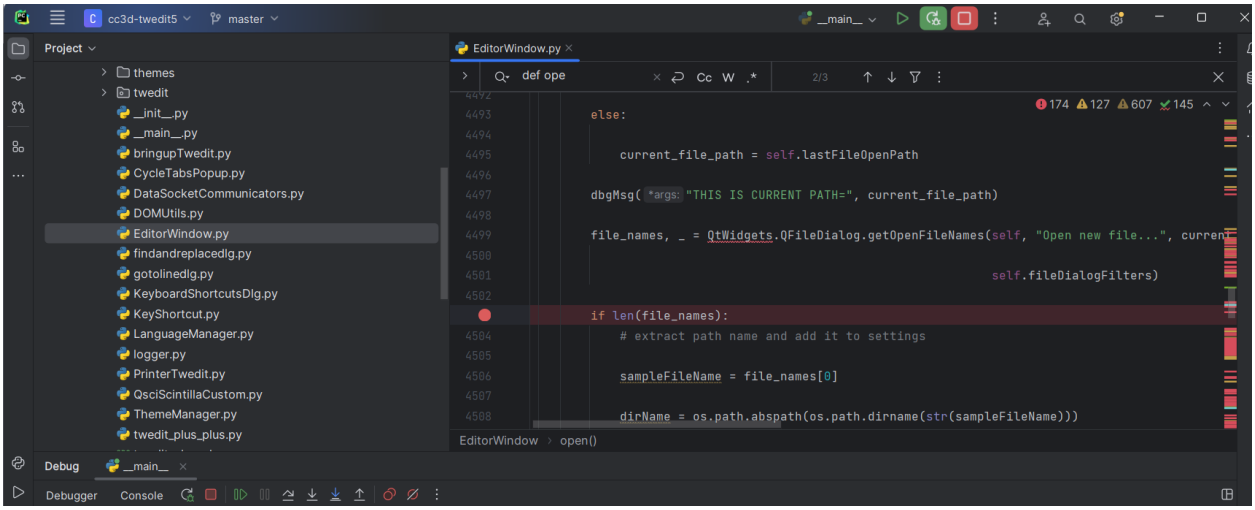
At this point if you are tired of clicking `F8` to step through the code let's click `Program Resume` and this will execute the rest of `loadFiles` function as well as the rest of `open` function that we were initially in.



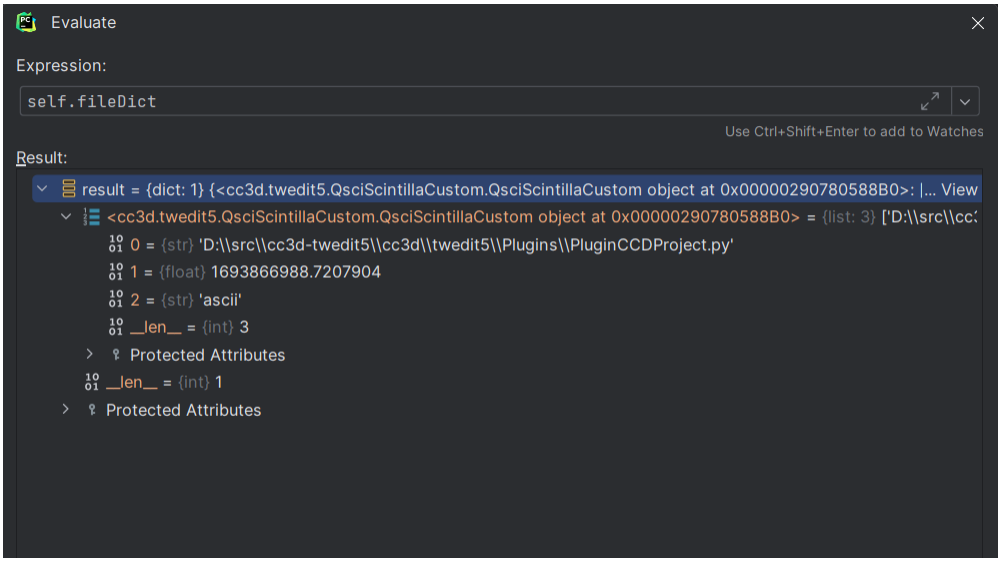
After you click `Resume Programs` you can switch to Twedit++ window and you will see that the file you selected is actually open now:



Finally, let's do another round of opening. But let's place another breakpoint after `lines`



Select `File->Open`, click `Resume Program` button to get past first breakpoint and we will get stopped at the second one . Open `Evaluate Expression` (`Alt-F8`) window and type `self.fileDict` in the entry line and hit `Enter`:



As you remember this variable was empty before we opened previous file. Now it is populated, the content is displayed above and we can conclude that it must have been populated during previous file open round. As an exercise you may want to find the place in the code where Twedit++ code inserts value into `self.fileDict`

This brief tutorial is an intro to debugging teaches you how to start exploring CompuCell3D UI in the debugger. Those skills are very helpful when developing UI code and once you learn how to use debugger effectively you will be using it quite a lot when you develop new UI modules. There are few skills that are useful during debugging: Setting up breakpoints, Evaluating expressions (`Alt-F8`), stepping over the code lines `F8`, stepping into the function `F7` and navigating the Call Stack. Once you learn those skills code development and learning what a given piece of code does will become a lot easier.

CHAPTER

TWENTYFOUR

INDICES AND TABLES

- genindex
- modindex
- search