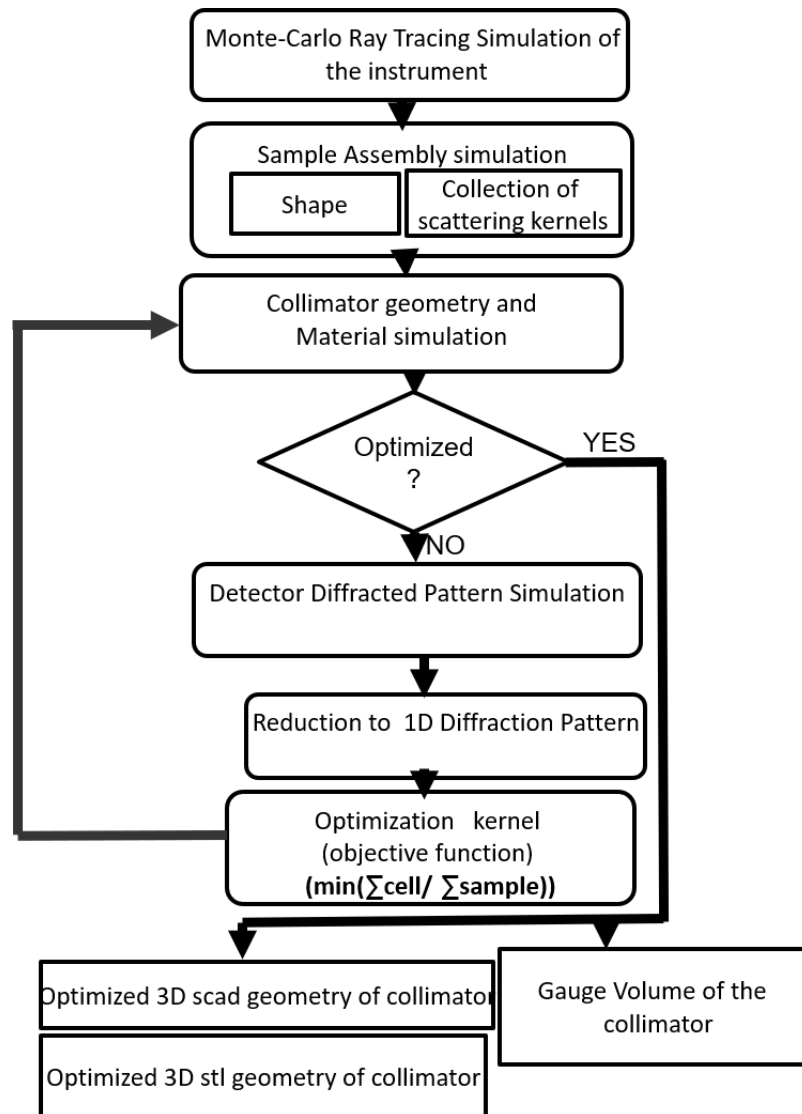# c3dp Documentation

Release 0.2.0

Fahima islam

Oct 09, 2019

Contents:

c3dp

1.1 Automated design of 3D printed collimator optimized for high pressure diffraction

1.2 Features

- Simulation of the the diffractometer (https://github.com/Fahima-Islam/McStas_SNAP)

- SImulation of the pressure cell (https://github.com/Fahima-Islam/c3dp/blob/master/docs/poster_ICANS.pdf)

- Optimization of the collimator for the given pressure cell

- Produced the .stl or .scad file of the collimator to be 3D printed (https://github.com/Fahima-Islam/c3dp/blob/master/docs/poster_ICANS.pdf)

- Produced the comparison in the diffraction pattern for with and without collimator

- Produced the gauge volume of the collimator

```
┌─────────────────────────────────┐
│ Monte-Carlo Ray Tracing Simulation of │
│         the instrument          │
└─────────────────────────────────┘
                 │
                 ▼
┌─────────────────────────────────┐
│   Sample Assembly simulation    │
│  ┌──────────┐ ┌──────────────┐  │
│  │  Shape   │ │ Collection of │  │
│  │          │ │scattering kernels│ │
│  └──────────┘ └──────────────┘  │
└─────────────────────────────────┘
                 │
                 ▼
┌─────────────────────────────────┐
│    Collimator geometry and      │
│      Material simulation        │
└─────────────────────────────────┘
                 │
                 ▼
           ╱ Optimized ╲         YES
          ╱      ?       ╲──────────►
           ╲            ╱
                 │ NO
                 ▼
┌─────────────────────────────────┐
│ Detector Diffracted Pattern Simulation │
└─────────────────────────────────┘
                 │
                 ▼
┌─────────────────────────────────┐
│  Reduction to 1D Diffraction Pattern │
└─────────────────────────────────┘
                 │
                 ▼
┌─────────────────────────────────┐
│      Optimization   kernel      │
│      (objective function)       │
│      (min(∑cell/ ∑sample))      │
└─────────────────────────────────┘

┌──────────────────────────────┐   ┌──────────────────────────┐
│Optimized 3D scad geometry of collimator│ │ Gauge Volume of the     │
└──────────────────────────────┘   │     collimator           │
┌──────────────────────────────┐   └──────────────────────────┘
│Optimized 3D stl geometry of collimator│
└──────────────────────────────┘
```
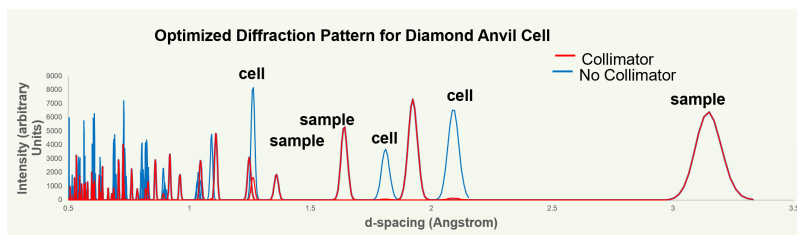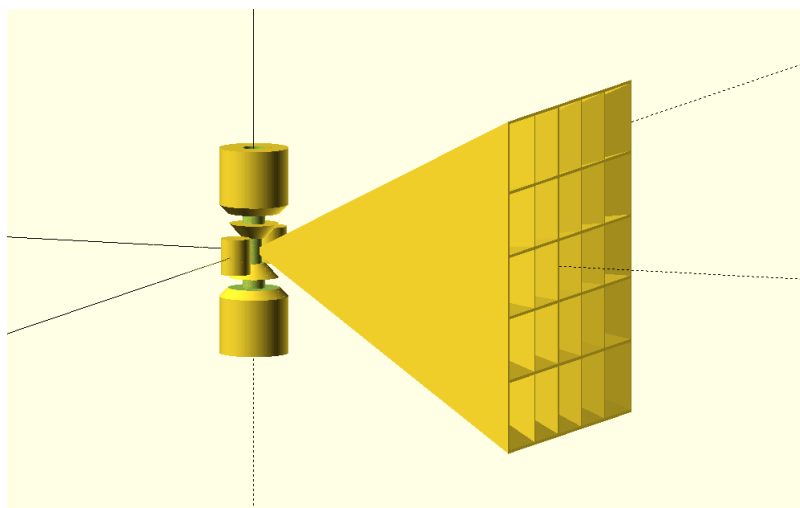
1.3 Examples

- Clamp cell:

Optimized Diffraction Pattern for Clamp Cell

- Diamond anvil cell:
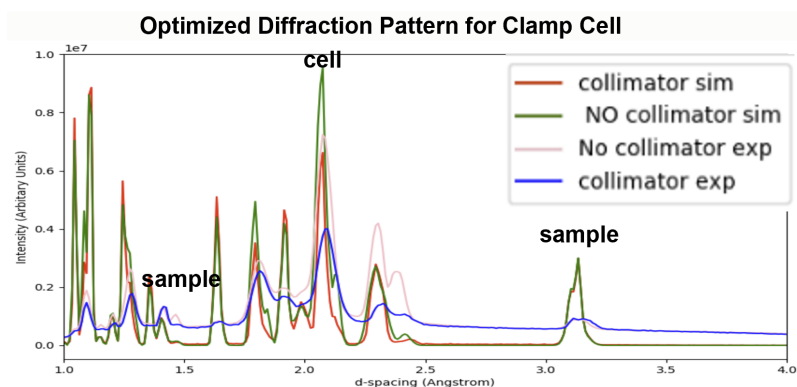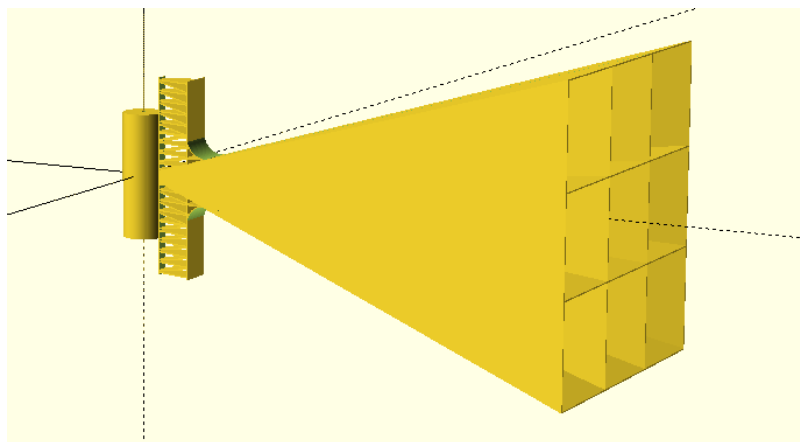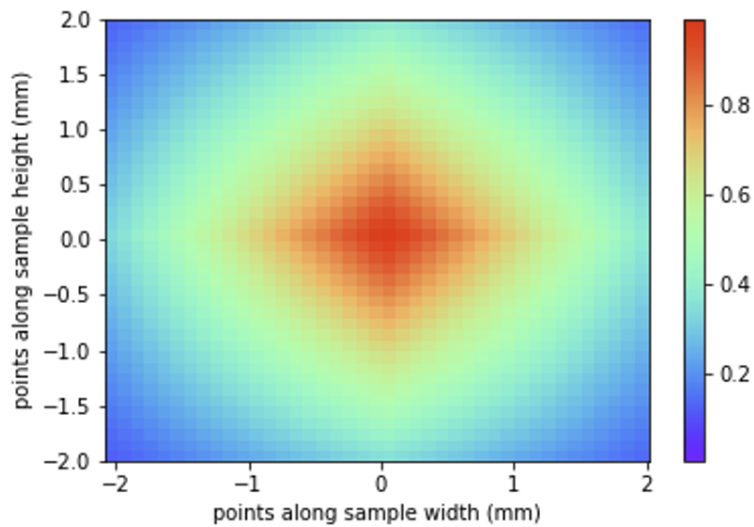

Optimized Diffraction Pattern for Diamond Anvil Cell

- Gauge volume:

gauge volume example: https://github.com/Fahima-Islam/c3dp/blob/gauge_volume/notebooks/gauge_volume.ipynb

1.4 Installation

- Clone the repository and execute from within and execute:

```
$ git clone git@github.com:Fahima-Islam/c3dp.git
$ cd c3dp
```

- Anaconda (Recommended)

```
$ conda install -c fi0 c3dp
```

- Pypi

```
$ pip install c3dp
```

Installation

2.1 Stable release

To install c3dp, run this command in your terminal:

```
$ pip install c3dp
```

This is the preferred method to install c3dp, as it will always install the most recent stable release.

If you don't have pip installed, this Python installation guide can guide you through the process.

2.2 From sources

The sources for c3dp can be downloaded from the Github repo.

You can either clone the public repository:

```
$ git clone git://github.com/fahima-islam/c3dp
```

Or download the tarball:

```
$ curl  -OL https://github.com/fahima-islam/c3dp/tarball/master
```

Once you have a copy of the source, you can install it with:

```
$ python setup.py install
```

Usage

To use c3dp in a project:

```python
import c3dp
```

Contributing

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given.

You can contribute in many ways:

4.1 Types of Contributions

4.1.1 Report Bugs

Report bugs at https://github.com/fahima-islam/c3dp/issues.

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

4.1.2 Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with "bug" and "help wanted" is open to whoever wants to implement it.

4.1.3 Implement Features

Look through the GitHub issues for features. Anything tagged with "enhancement" and "help wanted" is open to whoever wants to implement it.

4.1.4 Write Documentation

c3dp could always use more documentation, whether as part of the official c3dp docs, in docstrings, or even on the web in blog posts, articles, and such.

4.1.5 Submit Feedback

The best way to send feedback is to file an issue at https://github.com/fahima-islam/c3dp/issues.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

4.2 Get Started!

Ready to contribute? Here's how to set up *c3dp* for local development.

1. Fork the *c3dp* repo on GitHub.

2. Clone your fork locally:

```
$ git clone git@github.com:your_name_here/c3dp.git
```

3. Install your local copy into a virtualenv. Assuming you have virtualenvwrapper installed, this is how you set up your fork for local development:

```
$ mkvirtualenv c3dp
$ cd c3dp/
$ python setup.py develop
```

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

Now you can make your changes locally.

5. When you're done making changes, check that your changes pass flake8 and the tests, including testing other Python versions with tox:

```
$ flake8 c3dp tests
$ python setup.py test or py.test
$ tox
```

To get flake8 and tox, just pip install them into your virtualenv.

6. Commit your changes and push your branch to GitHub:

```
$ git add .
$ git commit -m "Your detailed description of your changes."
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

4.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

1. The pull request should include tests.

2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in README.rst.

3. The pull request should work for Python 2.7, 3.4, 3.5 and 3.6, and for PyPy. Check https://travis-ci.org/fahima-islam/c3dp/pull_requests and make sure that the tests pass for all supported Python versions.

4.4 Tips

To run a subset of tests:

```
$ py.test tests.test_c3dp
```

4.5 Deploying

A reminder for the maintainers on how to deploy. Make sure all your changes are committed (including an entry in HISTORY.rst). Then run:

```
$ bumpversion patch # possible: major / minor / patch
$ git push
$ git push --tags
```

Travis will then deploy to PyPI if tests pass.

Credits

5.1 Development Lead

- Fahima islam <ffiqnf.2017@gmail.com>

5.2 Contributors

None yet. Why not be the first?

History

6.1 0.1.0 (2019-04-22)

- First release on PyPI.

CHAPTER 7

Indices and tables

- genindex
- modindex
- search