TiltRec: An open-source tool that utilizes GPU acceleration for efficient tomographic reconstruction

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1 Overview

Here we present TiltRec, a GPU-accelerated tool for cryo-electron tomography reconstruction, designed for rapid and accurate three-dimensional reconstruction. TiltRec exhibits significant speed improvements compared to most current reconstruction software.

We provide users with four modes: y-axis non-accelerating, z-axis non-accelerating, y-axis slice-based accelerating, and z-axis unified memory accelerating. The y-axis and z-axis non-accelerating reconstruction mode supports three reconstruction methods: BPT, SIRT and SART. The y-axis slice-based accelerating reconstruction mode supports five methods: BPT, WBP, FBP, SIRT, and SART. The z-axis unified memory accelerating reconstruction mode supports six methods: BPT, WBP, FBP, SIRT, SART, and ADMM. TiltRec addresses the computational challenges in cryo-ET reconstruction, leveraging GPU acceleration to offer significant speed improvements. Additionally, it is fully open-source.

This manual introduces the instructions for installation (see section 2) and the detailed explanation of software parameters (see section 3).

2 Installation

The sections below explain how to download and install TiltRec on your computer.

2.1 Prerequisites

Note that TiltRec depends on and uses several external programs and libraries.

- Linux or Unix-like operating systems
- CMake
- OpenCV 4
- MPICH
- CUDA(Version above 11)

2.2 Installtion of TiltRec

We store the public release versions of TiltRec on GitHub, a site that provides code-development with version control and issue tracking through the use of git. To clone the repository, run the following command

```
git clone https://github.com/icthrm/TiltRec.git
```

For the convenience of environment configuration, we provide two compilation schemes: using Docker and not using Docker. Users who use Docker can directly install the external libraries described in Section 2.1 through Dockerfile, while users who do not use Docker must ensure that the server has correctly installed external libraries. The specific operations of both schemes are as follows:

- Using Docker

```
docker build -t tiltrec:v1 .
docker run -it --rm --gpus all tiltrec:v1 /bin/bash
cd build
cmake ..
make -j 8
```

- Not using Docker

```
cd build
cmake ..
make -j 8
```

2.3 Executable file description

After installation, four executable files will be generated, corresponding to four reconstruction modes, you can choose according to your needs:

- TiltRec-cuda: y-axis slice-based accelerating reconstruction

  Based on the y-axis acceleration reconstruction mode, it supports five methods: BPT, WBP, FBP, SIRT and SART. This mode divides the y-axis and uses GPU parallel processing, resulting in the fastest reconstruction speed and targeting practical users.

- TiltRec-mpi: y-axis non-accelerating reconstruction

  Based solely on the MPI-accelerated mode, it supports three methods: BPT,WBP,FBP, SIRT and SART. This mode divides the y-axis based on CPU reconstruction, improving reconstruction speed and targeting practical users.

- TiltRecZ-cuda: z-axis unified memory accelerating reconstruction

Based on the z-axis unified memory accelerating reconstruction mode, it supports six methods: BPT, WBP, FBP, SIRT, SART and ADMM. This mode has a slower speed compared to y-axis slice-based accelerating reconstruction and is aimed at method developers.

- TiltRecZ-mpi: z-axis non-accelerating reconstruction

Based solely on the MPI-accelerated mode, it supports three methods: BPT,WBP,FBP, SIRT,SART and ADMM. This mode does not segment the 3D body, resulting in a slower reconstruction speed and is aimed at method developers.

3 Explanation of parameters and examples

3.1 Parameter explanation of TiltRec

==== Required options ====

- --input(-i)

The name of the input MRC file used for reconstruction.

- --output(-o)

Designates the name of the resulting MRC file.

- --tiltfile(-t)

The file containing tilt angles for the reconstruction.

- --geometry(-g)

Defines geometric information of offset, pitch angle, z-axis offset, and thickness.

- --method(-m)

Selects the reconstruction method:

  - Back Projection: BPT
  - Filtered Back Projection: FBP
  - Weighted Back Projection: WBP
  - SART: SART, number of iterations, relaxation parameter
  - SIRT: SIRT, number of iterations, relaxation parameter

- ADMM: ADMM, number of iterations, number of conjugate gradient iterations, relaxation parameter, threshold

==== Optional options ====

- --initial

Provides an initial MRC file to be used as the model for iterative reconstruction methods.

- --help(-h)

Displays help information.

3.2 Explanation of output file

The output file is a 3D reconstruction result in MRC format, which can be opened and viewed in IMOD. The command is as follows:

```
imod outputfilename.mrc
```

3.3 Examples

When using TiltRec for 3D reconstruction, the necessary parameters provided by the user include the input MRC file, the resulting MRC file, the tilt angles file, the geometric information, and the reconstruction method. Other parameters are optional and users can choose according to their needs (see subsection 3.1). The following are four examples, corresponding to y-axis non-accelerating, y-axis slice-based accelerating, z-axis non-accelerating, and z-axis unified memory accelerating reconstruction.

- Example 1: y-axis non-accelerating reconstruction

```
mpirun -n 2 ./TiltRec-mpi --input ../../data/BBb/BBb_fin.mrc --output ../../
    data/BBb/BBb_output.mrc --tiltfile ../../data/BBb/BBb.rawtlt --geometry
    0,0,0,300 --method BPT
```

- Example 2: y-axis slice-based accelerating reconstruction

```
mpirun -n 2 ./TiltRec-cuda --input ../../data/BBb/BBb_fin.mrc --output ../../
    data/BBb/BBb_output.mrc --tiltfile ../../data/BBb/BBb.rawtlt --geometry
    0,0,0,300 --method WBP
```

- Example 3: z-axis non-accelerating reconstruction

```
mpirun -n 2 ./TiltRecZ-mpi --input ../../data/BBb/BBb_fin.mrc --output ../../
    data/BBb/BBb_output.mrc --tiltfile ../../data/BBb/BBb.rawtlt --geometry
    0,0,0,300 --method SIRT,10,0.2
```

- Example 4: z-axis unified memory accelerating reconstruction

```
./TiltRecZ-cuda --input ../../data/BBb/BBb_fin.mrc --output ../../data/BBb/
    BBb_output.mrc --tiltfile ../../data/BBb/BBb.rawtlt --geometry 0,0,0,300 --
    method SART,10,0.2
```