**GNU编译amber步骤：**

系统：Ubuntu16.04, amber18+ambertools18

**1. 依次安装以下包**

sudo apt-get install csh flex patch gfortran g++ make xorg-dev

sudo apt-get install libbz2-dev zlib1g-dev

sudo apt-get install libboost-dev libboost-thread-dev libboost-system-dev

**2. 解压安装包（假设amber安装在/home/test）**

cd /home/test

tar xvfj AmberTools18.tar.bz2

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1. **在bashrc文件里面写入amber安装路径：**
2. **gedit ~/.bashrc**

export AMBERHOME=/home/f/Amber/amber18

**4. 运行source ~/.bashrc,使环境变量生效**

**5. 编译串行版，依次运行以下命令：**

cd $AMBERHOME

./configure gnu

source amber.sh

make install

**6. 编译GPU版本**

6.1 下载cuda9.2，安装在默认路径（一般是/usr/local/cuda-9.2）

6.2 依次执行以下命令

export CUDA\_HOME=/usr/local/cuda-9.1

cd $AMBERHOME

./configure -cuda gnu

make install

1. **vim ~/.bashrc**

test -f /home/f/Amber/amber18/amber.sh && source /home/f/Amber/amber18/amber.sh