

APBS Roll: Users Guide

Rocks Version 4.3 Edition

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Preface

The main purpose of the APBS Roll is to install and configure the APBS¹ package on x86 or x86_64 based Rocks² clusters.

APBS (Adaptive Poisson-Boltzmann Solver)³ is a software package for the numerical solution of the Poisson-Boltzmann equation (PBE), one of the most popular continuum models for describing electrostatic interactions between molecular solutes in salty, aqueous media. APBS was designed to efficiently evaluate electrostatic properties for a wide range of length scales to enable the investigation of molecules with tens to millions of atoms.

The APBS Roll can be downloaded from the APBS download site⁴ and the Roll documentation including installation and usage information is available on the NBCR web site⁵.



The APBS Roll version number reflects version of Rocks for which this Roll is packaged, e.g., roll `apbs-4.3` will contain APBS for Rocks version 4.3.

The Roll is being developed by Robert Konecny <rok@ucsd.edu> with help from Greg Bruno, Nadya Williams, Todd Dolinsky and Nathan Baker.

Notes

1. <http://apbs.sourceforge.net/>
2. <http://www.rocksclusters.org>
3. <http://apbs.sourceforge.net/>
4. <http://sourceforge.net/projects/apbs>
5. <http://nbcrc.net/software/doc/apbs-roll/4.3>

Chapter 1. Requirements

1.1. APBS Version

This APBS Roll contains APBS version 0.5.1. The only changes with respect to the official APBS 0.5.1 release was addition of `pdb2pqr` package (version 1.2.1).

1.2. Rocks Version

This APBS Roll is for use with Rocks version 4.3 (Mars Hill).

1.3. Other Rolls

The APBS Roll does not require any other rolls, except the base Rocks roll.

Chapter 2. Installing the APBS Roll

2.1. Adding the Roll

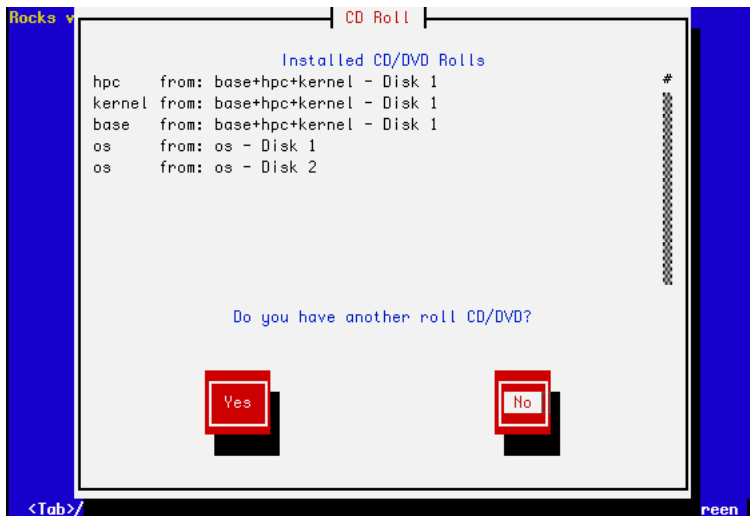
The APBS Roll is available for two different architectures: i386 and x86_64. Make sure you choose the correct iso image with the right APBS Roll for your specific hardware.

First please make sure you downloaded the iso images correctly (see MD5 checksums below) and then burn the iso image to a CD.

```
ee9aeacbfd30ee19061d14c97d67e38b  apbs-4.3-1.i386.disk1.iso
8133e93b29b3dcd570e6922f4c76511d  apbs-4.3-1.x86_64.disk1.iso
```

The APBS Roll can be installed during the Frontend installation step of your cluster (refer to section 1.2¹ of the Rocks users guide) but it can also be installed directly onto a running system.

The APBS Roll is added to a Frontend installation in exactly the same manner as other Rocks rolls. Specifically, after the base Roll is added the installer will once again ask if you have another Roll (see below). Select 'Yes' and insert a CD with the APBS Roll.



When you install the APBS Roll this way it will automatically be incorporated into the distribution for compute nodes in your cluster. This method the easiest and most natural way to install rolls in a Rocks cluster.

2.2. Adding the Roll to a Running Cluster

Starting with Rocks version 4.0.0 it is possible to add a Roll to a running cluster.

1. Installation of APBS on compute nodes.

Insert your APBS Roll CD into a Frontend CD/DVD drive and follow these steps:

```
# mount /mnt/cdrom
```

```
# cd /home/install
# rocks-dist --install copyroll
# umount /mnt/cdrom
# rocks-dist dist
```

and then reinstall compute nodes (using `kickstart` or `shoot-node` for example).



The iso image does not have to be burned onto a disk, it can be mounted on `/mnt/cdrom` instead:

```
# mount -o loop iso-image /mnt/cdrom
```

2. Installation of APBS on the Frontend.

Once you installed the APBS Roll on compute nodes the following steps will install it also on the frontend:

```
# kroll apbs > /tmp/install-apbs.sh
# sh -x /tmp/install-apbs.sh
```

After this, all APBS RPMs will be installed on the Frontend and available for users.



The above procedure works only for Rocks version 4.0.0 and later. However, it is possible to add individual APBS Roll RPMs to an older version of Rocks. Please follow directions in Chapter 2.2 in the APBS Roll documentation for Rocks 3.3.0.

After the installation, `apbs` executable is available in `/opt/apbs/bin` on the Frontend and all compute nodes. `/opt/apbs` directory on the Frontend and compute nodes also contains APBS documentation, examples, APBS tools and `pdb2pqr` package.

Technical details: The APBS i386 binary was compiled with Intel compilers version 10.0.023, MKL 9.1 and MPICH 1.2.7p1. The x86_64 APBS executable was compiled with Intel emt64 compiler version 10.0.023, MKL BLAS library version 9.1 and MPICH 1.2.7p1.

Notes

1. <http://www.rocksclusters.org/rocks-documentation/4.3/>

Chapter 3. Using the APBS Roll

3.1. How to use the APBS package

For detailed information on how to use APBS¹ please see APBS documentation² and APBS tutorial³.

In additions to tools available in `/opt/apbs/tools` directory you may find very useful the PDB2PQR web service⁴ which vastly simplifies preparation of APBS input files. Command line version of this utility is available in `/opt/apbs/pdb2pqr` as `pdb2pqr.py`.

For additional help there are two APBS mailing lists⁵: `apbs-users` and `apbs-announce`. The list archives are excellent source in case you have any problems using APBS.

3.2. Using APBS with SGE

If you wish to use APBS on the cluster together with SGE scheduling you can modify and use the following SGE script template:

```
#!/bin/csh -f
#$ -cwd
#
#$ -N apbs-PARALLEL
#$ -e apbs-PARALLEL.errout
#$ -o apbs-PARALLEL.errout
#
# requesting 8 processors
#$ -pe mpi 8
setenv NCPU 8

echo -n "Running on master node (using $NCPU CPUs): "
hostname

setenv APBSBIN /opt/apbs/bin/apbs
setenv MPIRUN /opt/mpich/gnu/bin/mpirun

echo "Starting apbs-PARALLEL calculation ..."

$MPIRUN -v -machinefile $TMPDIR/machines -np $NCPU \
    $APBSBIN apbs-PARALLEL.in >& apbs-PARALLEL.out

echo "Done."
```

Notes

1. <http://apbs.sourceforge.net/>
2. <http://apbs.sourceforge.net/doc/index.html>

3. <http://apbs.sourceforge.net/doc/tutorial/index.html>
4. <http://nbcv.net/pdb2pqr/>
5. <http://apbs.sourceforge.net/#lists>