

# UNRES server

- <http://ha1.chem.univ.gda.pl:8001/>
- <http://etoh.chem.univ.gda.pl:81/>

# UNRES web

[www.unres.pl](http://www.unres.pl)

# UNRES package installation

## UBUNTU

Requirements:

- 1) GIT
- 2) MPI
- 3) Cmake
- 4) Ifort/gfortran compiler
- 5) m4

# GIT

- `apt-get update`
- `apt-get upgrade`
- `apt-get install git`

# UNRES package download

- git clone

<http://mmka.chem.univ.gda.pl/repo/unres.git>

For UNRES4 (UCGM):

- git clone

<http://mmka.chem.univ.gda.pl/repo/unres4.git>

# Cmake

```
sudo apt-get install cmake
```

# Gfortran

```
sudo apt-get install gfortran
```

# m4

```
sudo apt-get install m4
```

# IF non-English UBUNTU VERSION

```
export LC_ALL=C
```

## Installation

```
cd unres
```

```
mkdir build
```

```
cd build
```

```
cmake ..
```

```
make -j4 (4 cores used to compile)
```

# Tests

## ctest

```
Start 36: WHAM_M_remd
36/48 Test #36: WHAM_M_remd ..... Passed 1.22 sec
Start 37: CLUSTER_WHAM_remd
37/48 Test #37: CLUSTER_WHAM_remd ..... Passed 0.74 sec
Start 38: CLUSTER_WHAM_M_remd
38/48 Test #38: CLUSTER_WHAM_M_remd ..... Passed 0.75 sec
Start 39: UNRES-MIN_ENE_protA
39/48 Test #39: UNRES-MIN_ENE_protA ..... Passed 0.06 sec
Start 40: UNRES-MIN_MIN_protA
40/48 Test #40: UNRES-MIN_MIN_protA ..... Passed 1.19 sec
Start 41: UNRES-MIN_MIN_INT
41/48 Test #41: UNRES-MIN_MIN_INT ..... Passed 0.17 sec
Start 42: CLUSTER_INT
42/48 Test #42: CLUSTER_INT ..... Passed 0.26 sec
Start 43: XDRF2PDB-one
43/48 Test #43: XDRF2PDB-one ..... Passed 0.00 sec
Start 44: XDRF2PDB-three
44/48 Test #44: XDRF2PDB-three ..... Passed 0.00 sec
Start 45: XDRF2PDB-M-one
45/48 Test #45: XDRF2PDB-M-one ..... Passed 0.01 sec
Start 46: XDRF2PDB-M-three
```

# Other branches

- AFM

(lipids, AFM, PBC, Nanotubes, Lorentzian-like restrains)

- Homology

(PBC, Homology restrains, Lorentzian-like restrains)