

## GROMACS Application Execution Guidelines for vSMP Foundation Aggregated Virtual Machine

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### Overview

GROMACS (Groningen Machine for Chemical Simulations) is a molecular dynamics simulation package originally developed in the University of Groningen(1). This document describes the best practice for running GROMACS 4.0 (from here on referred to as "GROMACS") on a vSMPowered system.

GROMACS uses MPI to communicate between its processes. The MPI library affects the way the application scales to large number of CPUs. The default MPI library which GROMACS ships with is MPICH-2.

### General Recommendations

If you haven't already done so, please read through "Execution Guidelines for vSMPowered Systems". This short document will provide you with recommendations that are not application-specific.

### Executing GROMACS

```
export MPIHOME=/opt/ScaleMP/mpich2/1.3.2
```

```
export PATH=$MPIHOME/bin:$PATH
```

```
export LD_LIBRARY_PATH=$MPIHOME/lib:$LD_LIBRARY_PATH
```

```
grompp_mpi -v -f grompp -o test_16 -c conf -p topol
```

```
mpiexec -np 16 mdrun_mpi -v -s test_16 -e test_16 -o test_16 -c after_test -g test_16 >& test_16.job
```

### Environment Variables – MPICH2

```
export VSMP_PLACEMENT=PACKED
```

```
export VSMP_MEM_PIN=YES
```

## Building fftw

fftw3 is available at (2).

```
#!/bin/sh

source /opt/intel/fce/latest/bin/ifortvars.sh intel64

source /opt/intel/cce/latest/bin/iccvars.sh intel64

BASE=`pwd`

tar xzf fftw-3.1.3.tar.gz

cd fftw-3.1.3

export CC=icc

export F77=ifort

export CXX=icpc

export F90=ifort

./configure --enable-float --enable-sse --prefix=${BASE}/fftw-sgl

make -j 16

make install
```

## Building GROMACS

```
#!/bin/sh

./opt/intel/Compiler/latest/bin/iccvars.sh intel64

./opt/intel/Compiler/latest/bin/ifortvars.sh intel64

export BASE=`pwd`
```

```
export GROMACSDIR=$BASE

export FFTWDIR=$GROMACSDIR/fftw-sgl

export FFTWFLAGS="-I$FFTWDIR/include -L$FFTWDIR/lib "

export CONFIG_INCLUDE="-I$GROMACSDIR/src"

export MPIPATH=/opt/ScaleMP/mpich2/1.3.2

export PATH=$MPIPATH/bin:$PATH

export MPICC='mpicc -cc=icc'

export CFLAGS=" -O3 -xHOST -fno-alias -fno-fnalias -g "

export CFLAGS="$CFLAGS $CONFIG_INCLUDE -I$FFTWDIR/include"

export LDFLAGS="-L$FFTWDIR/lib "

export AR=xiar

export CC=icc

export F77=ifort

export CXX=icpc

export F90=ifort

make distclean

./configure --with-fft=fftw3 --enable-mpi --program-suffix=_mpi --prefix=$BASE/gromacs4 || exit 1

make -j 8 || exit 1

make install || exit 1
```

## Footnotes

- (1) <http://en.wikipedia.org/wiki/GROMACS>.
- (2) <http://fftw.org>