

Jaguar 8 – Execution Guidelines for running applications in aggregated environment using ScaleMP’s vSMP Foundation

Overview

Jaguar is a multi-process application that uses MPI for inter-process communication. Open-MPI has been set as the default MPI for the Jaguar application. In addition Jaguar supports MPICH2 as well.

While it is possible to run Jaguar on the aggregation platform with any MPI implementation, using MPICH2 tuned for vSMP Foundation may yield a performance improvement of 5-15%.

In addition, it is recommended to run Jaguar with fast scratch using SW-RAID or ideally with a ram-drive.

Running Jaguar with MPICH2 tuned for vSMP Foundation

The original MPI implementation (OpenMPI) needs to be replaced by using Schrodinger MPI compatibility libraries for Linux.

The following steps are required:

1. Obtain the MPI compatibility library from ScaleMP (support@scalemp.com)
schrodinger_mpi.tar.gz
2. `cp schrodinger_mpi.tar.gz /tmp`
3. `cd /tmp`
4. Execute the script below to build the library for MPICH2.

```
----- Building libraries -----
#!/bin/sh

./opt/intel/Compiler/<version>/bin/iccvars.sh intel64
./opt/intel/Compiler/<version>/bin/fortvars.sh intel64
export MKL_HOME=/opt/intel/Compiler/<version>/mkl
export SCHRODINGER=/opt/schrodinger
export MPICH_HOME=/opt/ScaleMP/mpich2/1.0.8

rm -rf schrodinger_mpi
tar xzf schrodinger_mpi.tar.gz

cd schrodinger_mpi

sed -i -e "17i\SCHRODINGER = $SCHRODINGER" Makefile

sed -i -e "18i\MPI=MPICH" Makefile

sed -i -e "40i\ MPI_DIR = $MPICH_HOME" Makefile
```

```
sed -i -e "81i\SOURCE_BLACS_LIBS = $MKL_HOME/lib/em64t/libmkl_blacs_intelmpi_lp64.a" Makefile
sed -i -e "162i\    LIB_TARGETS = libcmp.so libprun.so" Makefile
sed -i -e "163d" Makefile
sed -i -e "s,MPI_LIB =.*,MPI_LIB = -L,$MPICH_HOME/lib -lmpich," Makefile
sed -i -e "s,BLACS_DIR =.*,BLACS_DIR = `pwd`/../../BLACS/LIB," Makefile
sed -i -e 's,CFLAGS =.*,CFLAGS = -fPIC -DBIND_ -DLINUX -I$(MPI_INCLUDE) ,' Makefile
sed -i -e "s,-lmpich -lmpich,-lmpich," Makefile
sed -i -e "87d" parallel_command.c
sed -i -e "87d" parallel_command.c
make install
```

----- Library build script -----

Environment variables – MPICH2

```
export VSMP_PLACEMENT=PACKED
export VSMP_MEM_PIN=YES
```

Running Jaguar with Ram-Drive

Since Jaguar jobs may perform a lot of scratch IO, setting TMPDIR to use a ram-drive, may yield shorter runtimes. In order to run with Ram-Drive, perform the following:

```
sudo mkdir /ramfs
sudo mount /dev/ram -t ramfs /ramfs -o noatime
sudo chmod 777 /ramfs
```

When launching Jaguar, add '-TMPDIR /ramfs ', in order to set the temporary directory used by the application.

NFS /home & /opt

Assuming Jaguar was installed under /opt, it turned out that some file I/O took place in \$HOME/.schrodinger and /opt/schrodinger.

If one of the directories is mounted over nfs, it may degrade the performance.

To avoid using NFS file system while running Jaguar, perform the following:

1. Find a partition in a local hard disk, such as /scratch
2. Set \$HOME to /scratch/<userid> (ie, export HOME=/scratch/<userid>)
3. cp -r /opt/schrodinger /scratch # if /opt is mounted over nfs
4. sudo amount /opt
5. sudo ln -s /scratch/schrodinger /opt/schrodinger

Sample script for MPICH2 tuned for vSMP

```
----- Jaguar run script -----
export SCHRODINGER=/opt/schrodinger
export MPICH_HOME=/opt/ScaleMP/mpich2/1.0.8

export PATH=${MPICH_HOME}/bin:$PATH

export LD_LIBRARY_PATH=$MPICH_HOME/lib:$LD_LIBRARY_PATH

export LD_LIBRARY_PATH=/opt/intel/Compiler/<version>/lib/intel64:/opt/intel/Compi
ler/<version>/mkl/lib/em64t:$LD_LIBRARY_PATH
export VSMP_PLACEMENT=PACKED
export VSMP_MEM_PIN=YES
ulimit -s unlimited

jaguar run -TMPDIR /ramfs -PROCS 16 <filename>.in
```

```
----- Jaguar run script -----
```

- **TMPDIR:** sets the temporary directory used by the application. For some workloads, it may be advantageous to have this temporary directory located on a fast disk device or even on /ramfs
- **PROCS 16:** sets the number of CPUs used by the application.
- **Make sure /ramfs** is mounted correctly as described above