Running ABAQUS jobs via Message Passing Interface (MPI)

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With the release of version 6 of the ABAQUS finite element analysis software, the developers have included MPI-based analysis for their Standard and Explicit solvers. In this article, details of the MPI-based analysis are presented and some benchmark results are included to show the improvements of the run times using this parallel analysis method. The benchmark was performed on SVU's Itanium2 servers running 1.5GHz IA64 processors.

Parallel Analysis in ABAQUS

ABAQUS had been developed with parallel programming features for a long time, but the parallel runs were only possible on shared-memory, multiprocessor systems prior to version 6 of the software. With the increasing popularity of cluster-based systems (SVU has several x86-based clusters since December 2002), the developers of the software have packaged a version of MPI (hpmpi) in their distribution CDs. The MPI packages are installed out of the box and will work independently of any other version of MPI installed on your clusters.

Requirements

As in all other MPI implementations, there are a few requirements for MPI to work:

- ability to launch programs on remote nodes via rsh or ssh - for SVU, ssh is used, and rsh is disabled for security purposes.
- high-speed, low-latency interconnects - traditional Ethernet-based interconnects will be much slower than the newer high-speed, low-latency interconnects such as quadrics, myrinet or infiniband. SVU has both myrinet and infiniband installed on selected clusters. For now, ABAQUS is not tested on myrinet or infiniband in SVU clusters, and only Ethernet connection is tested.

Setting up and Running MPI-based ABAQUS

To start using MPI, you will need to configure your ssh to allow you to launch jobs on a remote node of a cluster. There are many ways to do this, but SVU systems have been configured to set your account with a unique ssh key pair that will allow you to do this. If your account has not been set up properly, please contact our friendly support staff at ccesvuhelp@nus.edu.sg.
Next, you will need to determine which nodes you want to use for MPI runs and set this choice in your 'abaqus_v6.env' file, for example:

```bash
cpus=8
mp_host_list=[['cougar3',4],['cougar4',4]]
```

You will also need to specify the method of analysis using the `mp_mode` parameter as follows:

```bash
mp_mode=MPI
```

Note that this parameter can also be set to `mp_mode=THREADS` to run analysis in a traditional shared-memory multi-processor system.

To run an analysis, simply have the abaqus_v6.env in the same directory as the analysis input files, and issue the following command:

```bash
prompt> abaqus job=[input_file_name]
```

### Performance of Parallel Abaqus Runs using MPI

The benchmark example from ABAQUS, "A penny shaped crack under concentrated forces", was used to test the MPI performance. The three input files, namely, `ppennycrack.inp`, `ppennycrack_node.inp` and `ppennycrack_element.inp` were obtained from the example archives using the fetch option in the "abaqus" command. The following figure shows the speed up profile of the analysis job against the number of processors used.
From the figure shown above, the following can be observed:

- The time taken for the analysis to complete is shortened by approximately half using the MPI method.
- Increasing the number of processors is beneficial to the analysis run, up to 3 processors. Beyond this, there is no significant decrease in analysis run time. In fact, the time taken to complete the job increases slightly, possibly due to overheads in the communications between nodes.

Besides the above results, other benefits of MPI under ABAQUS were also discovered:

- The set up of an analysis job for MPI parallel run is simple, and does not require a user to modify their input files. Only parameters in the abaqus_v6.env environment file need to be changed or set to the correct values. When the abaqus_v6.env is set properly, the command to launch the analysis job is the same.
- MPI is supported for both Standard and Explicit jobs.
- The data files do not have to be transferred to the remote nodes. All directory and files required for the MPI run will be created or transferred over to the remote node automatically by ABAQUS, and the final results are consolidated at the head node.
- A major benefit seen in ABAQUS is that the MPI features are seamlessly integrated into the software and users do not have to learn MPI to be able to run it. Also, ABAQUS will automatically choose the MPI modules in the
analysis wherever the option is available when the mp_mode is set to MPI and ABAQUS will also report which parts of the analysis is not run using MPI.

For more detailed information on ABAQUS parallel jobs, please refer to the ABAQUS manuals.