TCAD Parallelization Environment Setup User Guide

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About This Guide

This user guide describes how to set up a parallelization environment for Synopsys® TCAD Sentaurus™ tools.

For additional information, see:

- The TCAD Sentaurus release notes, available on the Synopsys SolvNetPlus support site (see Accessing SolvNetPlus)
- Documentation available on the SolvNetPlus support site

Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
`Courier font`	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.
Italicized text	Used for emphasis, the titles of books and journals, and non-English words. It also identifies components of an equation or a formula, a placeholder, or an identifier.

Customer Support

Customer support is available through the Synopsys SolvNetPlus support site and by contacting the Synopsys support center.

Accessing SolvNetPlus

The SolvNetPlus support site includes an electronic knowledge base of technical articles and answers to frequently asked questions about Synopsys tools. The site also gives you access to a wide range of Synopsys online services, which include downloading software, viewing documentation, and entering a call to the Support Center.

To access the SolvNetPlus site:

1. Go to https://solvnetplus.synopsys.com.
2. Enter your user name and password. (If you do not have a Synopsys user name and password, follow the instructions to register.)

Contacting Synopsys Support

If you have problems, questions, or suggestions, you can contact Synopsys support in the following ways:

- Go to the Synopsys Global Support Centers site on www.synopsys.com. There you can find email addresses and telephone numbers for Synopsys support centers throughout the world.
- Go to either the Synopsys SolvNetPlus site or the Synopsys Global Support Centers site and open a case (Synopsys user name and password required).

Contacting Your Local TCAD Support Team Directly

Send an email message to:

- support-tcad-us@synopsys.com from within North America and South America
- support-tcad-eu@synopsys.com from within Europe
- support-tcad-ap@synopsys.com from within Asia Pacific (China, Taiwan, Singapore, Malaysia, India, Australia)
- support-tcad-kr@synopsys.com from Korea
- support-tcad-jp@synopsys.com from Japan

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Environment Setup

This chapter describes the setup for different parallelization strategies used by TCAD Sentaurus tools.

Overview of Parallelization

Several TCAD Sentaurus tools use parallelization to improve performance when they run on one of the following supported systems:

- *Shared-memory parallelization* (SMP) systems (usually referred to as multicores)
- *Distributed processing* (DP) systems (usually referred to as clusters)
- *Hardware-accelerated* systems (usually referred to as servers, each equipped with a dedicated hardware accelerator such as a graphics processing unit)

Some TCAD Sentaurus tools also use a combination of SMP, DP, and hardware-accelerated systems, which is referred to as mixed parallel mode.

Shared-Memory Parallelization

In general, no special setup is needed to run simulations using SMP.

Depending on the TCAD Sentaurus tool, you can specify the number of threads either on the command line or in the command file. In particular, all TCAD Sentaurus tools support the following command-line options:

- `--max_threads <i>`: This option sets the maximum number of threads that can be used in the simulation.
- `--threads <i>`: For Sentaurus Process and Sentaurus Interconnect, this option sets the default number of threads to use. For other tools, it sets the number of threads to use and overwrites any settings in the command file.

For tool-specific details, including the precedence rules of different options, refer to the respective documentation.

Parallelization Using the Message Passing Interface

In general, distributed computation by TCAD Sentaurus tools is implemented using the message passing interface (MPI) [1]. All tools use either the MPICH library [2] or the Intel® MPI Library [3] for the MPI implementation. Typically, separate processes are distributed over the cores of different server nodes, but you can also run all processes on the cores of a single node.

Distributing processes over a network of machines requires more setup steps than single-machine MPI simulations.

Installing TCAD Sentaurus on DP Systems

Setting up a distributed application is considerably more complex than setting up its serial or SMP version, because it requires an experienced system administrator with networking expertise on Linux operating systems.

You can try a preconfigured Linux cluster distribution such as Rocks before building a cluster [4].

Hardware and Software Setup

TCAD Sentaurus is available for Red Hat Enterprise Linux v7.3 on x86_64 platforms. All cluster nodes must be configured with a Synopsys QSC-compliant Linux distribution.

All nodes of the cluster should have the same software setup including the operating system version and TCAD Sentaurus tool version. You should install TCAD Sentaurus on a shared network drive that is accessible using the same path on all nodes. This configuration reduces potential sources of errors due to inconsistent software versions and configuration issues.

Note:

Some TCAD Sentaurus tools might require a cluster to have one head node that has more CPU power and RAM than the computing nodes, because the master process might require maximum RAM for all computed results and maximum CPU power for not yet DP-parallelized portions of the tool.

The overall speed of a TCAD Sentaurus tool is usually limited by the slowest node. The communication bandwidth between nodes can also affect significantly the overall performance, depending on the amount of data exchanged over the network for a specific tool.

Installing Clusters

To install a cluster:

1. Ensure the prerequisites for running a TCAD Sentaurus tool in DP parallel mode are met:
   a. SSH is installed on each system and is available in the search path of each user.
   b. Use a network file system for the installation and user directories, where the path will be the same for all nodes.
2. Install the TCAD Sentaurus distribution in the target directory on your network file system following the instructions in the *TCAD Installation Notes*.
3. Ensure each user has the correct environment settings to run TCAD Sentaurus, following the instructions in the *TCAD Installation Notes*.

Running TCAD Sentaurus Tools on a Cluster

You can run a TCAD Sentaurus tool on a cluster using plain Linux, MPI, and tool-specific commands.

In its simple form, to perform a simulation in DP parallel mode, you should:

1. Configure SSH for a password-less log-on to all required hosts. See Configuring SSH on page 9.
2. Create a file with a list of required hosts. The file must also include the head node on which the master process runs. See Creating the MPI Host File on page 10.
3. Run the TCAD Sentaurus tool. See Automatically Executing an MPI Simulation on a Cluster Using Command-Line Options on page 10.

   Note:

   Steps 1 and 2 are required only if you run a simulation on more than one node. For best performance, the number of processes requested on each node must not exceed the number of cores available on the node.

   Step 1 is required only once for each cluster; whereas, adapting the host file might be necessary if additional or different computational resources are required for a specific simulation.

You can also run a TCAD Sentaurus tool on a cluster using Sentaurus Workbench (see Parallel Job Control Using Sentaurus Workbench on page 12).

Configuring SSH

TCAD Sentaurus uses `mpiexec.hydra` from the MPICH library or the Intel MPI Library as the MPI process manager. As such, you must ensure that password-less SSH command invocations work from the head node to all computing nodes in a cluster.

Assuming a standard SSH installation and a shared home directory on all cluster nodes, you configure SSH by logging on to any of the cluster nodes as follows:

1. Generate a pair of authentication keys on the host:

   ```
   ssh-keygen -t rsa
   ```

2. Enter an empty passphrase by pressing the Enter key when asked for the passphrase, and use the default file name.

3. Add the public key to the authorized keys:

   ```
   touch ~/.ssh/authorized_keys

   chmod 600 ~/.ssh/authorized_keys

   cat ~/.ssh/id_rsa.pub >> ~/.ssh/authorized_keys
   ```

For alternatives, refer to the SSH documentation.

Use the following UNIX commands to verify that log-on without a password is possible for each relevant node with the name `<nodename>`:

```
ssh <nodename> hostname
```

If necessary, answer the question about the *RSA key fingerprint* with yes.

Moreover, the same commands should display the name of the cluster node without requiring any passwords, passphrases, RSA keys, or other input:

```
ssh <nodename> hostname
```

Alternative configurations include:

- The system administrator can provide you with a preconfigured `~/.ssh/known_hosts` file to avoid the *RSA key fingerprint* question.
- You can provide a suitable `/etc/ssh/known_hosts` file on each system.
- You can use the `ssh-keyscan` command to collect the necessary keys.

For more information about SSH configurations, see the SSH and SSHD documentation [5].

Creating the MPI Host File

The MPI host file lists the names of all the nodes of your cluster.

Note:

The host file must not contain empty lines.

For example, the `mpihostfile.txt` host file has the following content:

```
$ cat ~/mpihostfile.txt
node1:4
node2:4
node3:4
node4:4
```

In the example, if the total number of requested processes is 16, then four MPI processes must run on each of the four nodes. More precisely, the first four processes will run on host `node1`, the next four processes will run on host `node2`, and so on.

If only a list of nodes is specified, then `mpiexec.hydra` tries to divide the processes equally among the specified nodes in a round-robin manner.

In the following example, the `mpihostfile.txt` file is used for a simulation using 16 processes:

```
$ cat ~/mpihostfile.txt
node1
node2
node3
node4
```

The first and fifth processes will run on host `node1`, the second and the sixth processes will run on host `node2`, and so on.

Automatically Executing an MPI Simulation on a Cluster Using Command-Line Options

After successfully completing Steps 1 and 2 (see Running TCAD Sentaurus Tools on a Cluster on page 8) and verifying the MPI setup (see Verifying the MPI Setup on page 13), it is recommended to run the TCAD Sentaurus tool in DP parallel mode using the command-line option `--processes` from either the command line or Sentaurus Workbench.

You can use the following command to start a TCAD Sentaurus tool from the command line:

```
$ <tool_name> --processes <#processes>
   [--max_threads <max_#threads_per_process>]
   [--mpi-file <hostfile>]
   [--ssh-check yes | no]
   [--threads <#threads_per_process>]
```

```
[--mpi-type mpich | intel]
[--mpi-master-host <hostname>]
[<tool_command_line_options>] <command_file>
```

By default, all hosts in the host file will be tested for a silent SSH log-in before the MPI job starts. You can omit this check by specifying `--ssh-check no`.

For more information about the `--max_threads` and `--threads` command-line options, see Shared-Memory Parallelization on page 6.

For the format of the host file, see Creating the MPI Host File on page 10.

The option `--mpi-type` specifies which MPI installation is used to run the MPI simulation. The default is MPICH (`mpich`), but you could also specify Intel MPI (`intel`).

The MPI master host is used for dynamic MPI if it applies to your simulation task. This option is available only for tools that support MPI-2 dynamic process management, such as Raphael™ FX.

The advantage of automated cluster execution is that it manages MPI processes and the execution of `mpiexec.hydra` with the required command-line options (see Executing an MPI Simulation on a Cluster Using Low-Level MPI Commands).

Executing an MPI Simulation on a Cluster Using Low-Level MPI Commands

In the following situations, it might be necessary to use low-level MPI commands to run a TCAD Sentaurus tool on a cluster:

- Access to a cluster is granted only through a cluster management system.
- Additional MPI options must be set that are not supported by automated cluster execution using tool command-line options.
- You need to troubleshoot the MPI setup.

TCAD Sentaurus uses `mpiexec.hydra` from the MPICH library [2] or the Intel MPI Library [3] for process management and communication between nodes.

Note:

The MPICH library requires Python version 2.3 or higher for execution.

A compiled version of MPICH is installed with TCAD Sentaurus in the installation directory `$STROOT/tcad/current/linux64/tcad_mpi_mpich`, including binaries, man pages, and documentation as provided by MPICH.

A compiled version of Intel MPI is installed with TCAD Sentaurus in the installation directory `$STROOT/tcad/current/linux64/tcad_mpi_intel/intel64/`, including binaries, man pages, and documentation as provided by Intel MPI.

To make MPICH or Intel MPI available, you must configure the environment as follows:

1. Include the paths to both the TCAD Sentaurus tool supporting MPI and MPICH (or Intel MPI) in the `$PATH` variable.
2. Verify the correct settings by executing the following commands:

```
$ which <tool_name>
$ which mpiexec.hydra
```

Note:

Ensure the `$PATH` variable does not point to LAM MPI, Open MPI, and other MPI installations that might already exist on the system.

Hardware Acceleration Using Graphics Processing Units

Only Sentaurus Device Electromagnetic Wave Solver supports hardware acceleration using graphics processing units (GPUs).

See *Sentaurus™ Device Electromagnetic Wave Solver User Guide*, Chapter 9.

Parallel Job Control Using Sentaurus Workbench

Sentaurus Workbench provides special functionality that controls the submission of parallel jobs on both SMP and DP systems. It helps with the allocation of parallel resources, including the distribution of MPI processes according to different policies.

See *Sentaurus™ Workbench User Guide*, Configuring the Execution of Jobs.

References

[1] For more information, go to https://www.mpi-forum.org.

[2] For more information, go to https://www.mpich.org.

[3] For more information, go to https://www.intel.com/content/www/us/en/developer/tools/oneapi/mpi-library.html#gs.mutazs.

[4] For more information, go to http://www.rocksclusters.org.

[5] For more information, go to http://www.openssh.com.

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Message Passing Interface

This appendix describes how to verify the setup for the message passing interface (MPI).

Verifying the MPI Setup

To verify that the MPI setup is correct:

1. Ensure that the location of the MPICH library or Intel MPI Library installed with TCAD Sentaurus is in your `$PATH` variable, before any other MPI implementations, by executing the following command:

   ```
   $ which mpiexec.hydra
   ```

   Your path can be set in Bash using:

   ```
   $ export PATH=$STROOT/tcad/current/linux64/mpich/bin:${PATH}
   ```

   Your path can be set in C shell using:

   ```
   $ setenv PATH $STROOT/tcad/current/linux64/mpich/bin:${PATH}
   ```

2. Check that you can run a command multiple times on the local node:

   ```
   $ mpiexec.hydra -n 10 hostname
   ```

3. If this succeeds, run the TCAD Sentaurus tool supporting MPI with multiple workers on one node:

   ```
   $ mpiexec.hydra -n 8 <tool_name> <command_file>
   ```

4. Ensure that all hosts listed in the MPI host file (`<hostfile>`) run the TCAD Sentaurus tool correctly. Execute a command on all nodes specified in the host file:

   ```
   $ mpiexec.hydra -f <hostfile> hostname
   ```

   If the command freezes or generates error messages, then locate the cause by subsequent removal of host names from the file, and then return to Step 2 for that particular host.

5. Start the TCAD Sentaurus tool supporting MPI on the nodes specified in the host file:

```
$ mpiexec.hydra -n <#processes> -f <hostfile> <tool_name>
   <command_file>
```

If all commands execute successfully, then the system should be set up correctly to run the TCAD Sentaurus tool on a cluster.

Glossary

DP
Distributed processing.

GPU
Graphics processing unit.

Intel MPI Library
Library that implements the open-source MPI specification.

LAM MPI
Local area multicomputer message passing interface.

MPI
Message passing interface.

MPICH
Library that implements the open-source MPI specification.

mpiexec.hydra
MPI process manager.

Open MPI
An implementation of the MPI.

QSC
Qualified system configuration. The Synopsys Platforms Core Team defines and communicates the standard system configurations for the build and release environment for all Synopsys products. The environment is documented as the QSC and is part of the corresponding foundation.

SMP
Shared-memory parallelization.

SSH
Secure shell.

SSHD
OpenSSH daemon that runs and allows users to connect to a server.