# Contents

## Front Matter
1.1 Contact .......................................................... 1
1.2 Copyright ......................................................... 1
1.3 Documentation License ......................................... 1
1.4 Disclaimer ....................................................... 1
1.5 Trademark ....................................................... 2

## Release Notes
2.1 Introduction .................................................... 3
2.2 Release 1.4.0 (May 27, 2019) .................................. 3
2.3 Release 1.3.0 (May 18, 2019) ................................ 3
  2.3.1 Python 3 Examples ........................................ 3
  2.3.2 Tcl Support Deprecated .................................. 3
  2.3.3 Binary Releases .......................................... 4
2.4 Release 1.2.0 (May 8, 2019) ................................. 4
2.5 Release 1.1.0 (April 30, 2019) .............................. 4
2.6 Release 1.0.0 (December 18, 2018) ....................... 5
  2.6.1 Documentation ............................................ 5
  2.6.2 Version .................................................... 5
  2.6.3 Operating Systems ...................................... 5
  2.6.4 Python Support .......................................... 5
  2.6.5 GMSH Support ........................................... 6
  2.6.6 CGNS Support ............................................ 6
2.7 July 20, 2018 .................................................... 6
  2.7.1 Documentation ............................................ 6
  2.7.2 Python 3 Support ........................................ 7
  2.7.3 Element Information ..................................... 7
  2.7.4 Interface Boundary Condition .......................... 7
  2.7.5 Interface Equation Coupling ............................ 7
  2.7.6 Interface and Contact Surface Area ................... 7
  2.7.7 Bug Fixes .................................................. 7
<table>
<thead>
<tr>
<th>Date</th>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>May 15, 2017</td>
<td>2.8 May 15, 2017</td>
</tr>
<tr>
<td>November 24, 2015</td>
<td>2.10 November 24, 2015</td>
</tr>
<tr>
<td>November 1, 2015</td>
<td>2.11 November 1, 2015</td>
</tr>
<tr>
<td>September 6, 2015</td>
<td>2.12 September 6, 2015</td>
</tr>
<tr>
<td>August 10, 2015</td>
<td>2.13 August 10, 2015</td>
</tr>
<tr>
<td>June 7, 2015</td>
<td>2.15 June 7, 2015</td>
</tr>
<tr>
<td>October 4, 2014</td>
<td>2.16 October 4, 2014</td>
</tr>
<tr>
<td>December 25, 2013</td>
<td>2.17 December 25, 2013</td>
</tr>
<tr>
<td>September 8, 2013</td>
<td>2.18 September 8, 2013</td>
</tr>
<tr>
<td>August 14, 2013</td>
<td>2.19 August 14, 2013</td>
</tr>
<tr>
<td>July 29, 2013</td>
<td>2.20 July 29, 2013</td>
</tr>
</tbody>
</table>

3 Introduction

<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1 Overview</td>
</tr>
<tr>
<td>3.2 Goals</td>
</tr>
<tr>
<td>3.3 Structures</td>
</tr>
<tr>
<td>3.4 Equation assembly</td>
</tr>
<tr>
<td>3.5 Parameters</td>
</tr>
</tbody>
</table>
12.4 Source code availability ........................................... 56
12.5 Directory Structure ................................................ 56
12.6 Running DEVSIM ................................................... 56

13 Additional Information .............................................. 57
  13.1 DEVSIM License .................................................. 57
  13.2 SYMDIFF .......................................................... 57
  13.3 External Software Tools ........................................ 57
    13.3.1 Genius ....................................................... 57
    13.3.2 Gmsh ........................................................ 57
    13.3.3 Paraview ..................................................... 57
    13.3.4 Tecplot ...................................................... 58
    13.3.5 VisIt ........................................................ 58
  13.4 Library Availability ............................................. 58
    13.4.1 BLAS and LAPACK ........................................... 58
    13.4.2 CGNS ........................................................ 58
    13.4.3 Python ....................................................... 58
    13.4.4 SQLite3 ...................................................... 58
    13.4.5 SuperLU ...................................................... 58
    13.4.6 Tcl .......................................................... 59
    13.4.7 zlib ........................................................ 59

14 Command Reference .................................................. 61
  14.1 Circuit Commands ................................................ 61
  14.2 Equation Commands .............................................. 62
  14.3 Geometry Commands ............................................. 66
  14.4 Material Commands ............................................. 67
  14.5 Meshing Commands ............................................... 70
  14.6 Model Commands ................................................. 76
  14.7 Solver Commands ................................................ 88

15 Example Overview ................................................... 91
  15.1 capacitance ....................................................... 91
  15.2 diode ............................................................ 91
  15.3 bioapp1 .......................................................... 91
  15.4 genius ........................................................... 91
  15.5 vector_potential ................................................ 92
  15.6 mobility .......................................................... 92

16 Capacitor ............................................................. 93
  16.1 Overview .......................................................... 93
  16.2 1D Capacitor ...................................................... 93
    16.2.1 Equations .................................................... 93
    16.2.2 Creating the mesh ......................................... 93
  16.3 Setting device parameters ..................................... 94
    16.3.1 Creating the models ....................................... 94
    16.3.2 Contact boundary conditions ................................ 95
    16.3.3 Setting the boundary conditions ......................... 96
List of Figures

4.1 Mesh elements in 2D. .............................................. 20
4.2 Edge model constructs in 2D. ..................................... 21
4.3 Element edge model constructs in 2D. .......................... 22
4.4 Interface constructs in 2D. Interface node pairs are located at each ●. The SurfaceArea model is used to integrate flux term models. .......................... 27
4.5 Contact constructs in 2D. ........................................... 29

15.1 Simulation result for solving for the magnetic potential and field. The coloring is by the Z component of the magnetic potential, and the stream traces are for components of magnetic field. .................................................. 92

16.1 Capacitance simulation result. The coloring is by Potential, and the stream traces are for components of ElectricField. .................................................. 102

17.1 Carrier density versus position in 1D diode. ................ 106
17.2 Potential and electric field versus position in 1D diode. ......................... 107
17.3 Electron and hole current and recombination. ................ 108
### List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Contact</td>
<td>1</td>
</tr>
<tr>
<td>4.1</td>
<td>Node models defined on each region of a device.</td>
<td>23</td>
</tr>
<tr>
<td>4.2</td>
<td>Edge models defined on each region of a device.</td>
<td>24</td>
</tr>
<tr>
<td>4.3</td>
<td>Element edge models defined on each region of a device.</td>
<td>25</td>
</tr>
<tr>
<td>4.4</td>
<td>Required derivatives for equation assembly. <em>model</em> is the name of the model being evaluated, and <em>variable</em> is one of the solution variables being solved at each node.</td>
<td>25</td>
</tr>
<tr>
<td>4.5</td>
<td>Required derivatives for interface equation assembly. The node model name <em>nodemodel</em> and its derivatives <em>nodemodel:variable</em> are suffixed with @r0 and @r1 to denote which region on the interface is being referred to.</td>
<td>26</td>
</tr>
<tr>
<td>5.1</td>
<td>Parameters controlling program behavior.</td>
<td>34</td>
</tr>
<tr>
<td>10.1</td>
<td>Basic expressions involving unary, binary, and logical operators.</td>
<td>48</td>
</tr>
<tr>
<td>10.2</td>
<td>Predefined Functions.</td>
<td>49</td>
</tr>
<tr>
<td>10.3</td>
<td>Commands.</td>
<td>50</td>
</tr>
<tr>
<td>10.4</td>
<td>Commands for user functions.</td>
<td>50</td>
</tr>
<tr>
<td>12.1</td>
<td>Current platforms for DEVSIM.</td>
<td>55</td>
</tr>
<tr>
<td>12.2</td>
<td>Directory structure for DEVSIM.</td>
<td>56</td>
</tr>
<tr>
<td>17.1</td>
<td>Python package files.</td>
<td>103</td>
</tr>
</tbody>
</table>
Chapter 1

Front Matter

1.1 Contact

Table 1.1: Contact

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Web:</td>
<td><a href="https://devsim.com">https://devsim.com</a></td>
</tr>
<tr>
<td>Email:</td>
<td><a href="mailto:info@devsim.com">info@devsim.com</a></td>
</tr>
<tr>
<td>Open Source Project:</td>
<td><a href="https://devsim.org">https://devsim.org</a></td>
</tr>
<tr>
<td>Online Documentation:</td>
<td><a href="https://devsim.net">https://devsim.net</a></td>
</tr>
<tr>
<td>Online Forum:</td>
<td><a href="https://groups.google.com/d/forum/devsim">https://groups.google.com/d/forum/devsim</a></td>
</tr>
</tbody>
</table>

1.2 Copyright

Copyright © 2009–2018 DEVSIM LLC

1.3 Documentation License

This work is licensed under the Creative Commons Attribution-NoDerivatives 4.0 International License. To view a copy of this license, visit http://creativecommons.org/licenses/by-nd/4.0/.

1.4 Disclaimer

DEVSIM LLC MAKES NO WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, WITH REGARD TO THIS MATERIAL, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE.
1.5 Trademark

DEVSIM is a registered trademark and SYMDIFF is a trademark of DEVSIM LLC. All other product or company names are trademarks of their respective owners.
Chapter 2

Release Notes

2.1 Introduction

DEVSIM download and installation instructions are located in Installation (page 55). The following sections list bug fixes and enhancements over time. Contact information is listed in Contact (page 1).

2.2 Release 1.4.0 (May 27, 2019)

The devsim.custom_equation() (page 63) and devsim.register_function() (page 85) commands take Python functions, instead of the a string with the function name.

The following commands are available to store data on edges and element edges:

- edge_solution()
- set_edge_values()
- element_solution()
- set_element_values()

2.3 Release 1.3.0 (May 18, 2019)

2.3.1 Python 3 Examples

All of the Tcl regression tests in the testing directory have been converted to Python 3. These tests serve as examples for features that were previously only tested using Tcl scripting.

2.3.2 Tcl Support Deprecated

Tcl support is deprecated and will be removed in a future release of the software.
2.3.3 Binary Releases

Scripting Languages

Python 3 is now the only scripting language in the releases available from:
https://github.com/devsim/devsim/releases

Math Library

The Microsoft Windows version now uses Intel MKL Pardiso for direct matrix factorization. Both Linux and Apple macOS have been using Intel MKL Pardiso since November 1, 2015 (page 9). Binary releases for all operating systems use BLAS/LAPACK routines from Intel Math Kernel Library.

2.4 Release 1.2.0 (May 8, 2019)

DEVSIM releases have better support for Python 3. Using the stable ABI, the software is able to run newer Python 3 releases, without rebuilding the software.

Support for Python 2.7 has been removed.

The banner has been removed when the DEVSIM module is imported.

The symdiff python module is now part of the DEVSIM release. This module has additional features not available using the \texttt{devsim.symdiff()} (page 86) command from DEVSIM. By first setting the \texttt{PYTHONPATH} variable to the \texttt{lib} directory in the DEVSIM distribution, symdiff is loaded by using

\begin{verbatim}
import symdiff
\end{verbatim}

Documentation is available in the \texttt{doc} directory of this distribution. Examples are available in the \texttt{examples/symdiff} directory.

2.5 Release 1.1.0 (April 30, 2019)

The Bernoulli function, $B(x)$,

$$B(x) = \frac{x}{e^x - 1}$$

and its derivative,

$$dBdx(x) = \frac{e^x - 1 - xe^x}{(e^x - 1)^2}$$

have been refactored. They are used to calculate electron and hole current densities using the Scharfetter-Gummel method [SG69].
The Bernoulli function has numerical issues when $x$ approaches 0 and requires special evaluation. In this release, DEVSIM, takes advantage of C++11 math library functions for evaluating the denominator.

In addition, these functions are evaluated with extended precision, when this mode is enabled in the simulator. This mode is described in *Extended Precision* (page 7) and controlling parameters are in *Parameters controlling program behavior*. (page 34).

Users should expect that simulation results should change in the number of solver iterations and small differences in simulation results. This and other functions are listed in *Predefined Functions*. (page 49).

### 2.6 Release 1.0.0 (December 18, 2018)

#### 2.6.1 Documentation

The formatting of the PDF and online documentation has been improved. Also significant changes have been made to the way DEVSIM is called from Python.

#### 2.6.2 Version

Due to the numerous changes in the Python API, the version number has been updated to having a major revision of 1. We adopt the semantic version numbering presented at https://semver.org. The version number can be accessed through the Python interface using the `devsim.__version__` variable.

#### 2.6.3 Operating Systems

The Microsoft Windows 32-bit operating system is now supported in addition to the platforms listed in *Supported platforms* (page 55).

#### 2.6.4 Python Support

DEVSIM is now loaded as a shared library from any compatible Python interpreter. Previously, DEVSIM binaries contained an embedded Python interpreter. The following versions of Python are supported in this release

- 2.7
- 3.6
- 3.7

By first setting the `PYTHONPATH` variable to the `lib` directory in the DEVSIM distribution, `devsim` is loaded by using

```python
import devsim
```

from Python. Previous releases of devsim used the `ds` module, the manual will be updated to reflect the change in module name.
Many of the examples in the distribution rely on the `python_packages` module, which is available by using:

```python
import devsim.python_packages
```

The default version of Python for use in scripts is Python 3.7. Scripts written for earlier versions of Python 3 should work. Python 2.7 is deprecated for future development.

Anaconda Python 3.7 is the recommended distribution and is available from https://continuum.io. The Intel Math Kernel Library is required for the official DEVSIM releases. These may be installed in Anaconda using the following command:

```bash
conda install mkl
```

On the Microsoft Windows platform, the following packages should also be installed:

```bash
conda install sqlite zlib
```

Some of the examples and tests also use `numpy`, which is available using:

```bash
conda install numpy
```

Please see `User Interface` (page 43) and `Installation` (page 55) for more information.

### 2.6.5 GMSH Support

Gmsh has announced a new version of their mesh format 4.0. DEVSIM currently supports the previous version, 2.2. To load a file from Gmsh, it is now necessary to either:

- Save the file in the 2.2 format from Gmsh
- Parse the 4.0 file, and then use Custom mesh loading using scripting (page 40)

A future release of DEVSIM will provide this capability.

### 2.6.6 CGNS Support

Support for loading CGNS files is deprecated, and is no longer part of the official releases. Please see Using an external mesher (page 39) for more information about importing meshes from other tools.

### 2.7 July 20, 2018

#### 2.7.1 Documentation

The documentation has a new license, which is described in Copyright (page 1). The source files are now available for download from: https://github.com/devsim/devsim_documentation.
2.7.2 Python 3 Support

Python 3 executable, devsim_py3 is now supplied in addition to standard Python 2 executable, devsim.

2.7.3 Element Information

The devsim.get_element_node_list() (page 67) retrieves a list of nodes for every element on a region, contact, or interface.

2.7.4 Interface Boundary Condition

The type=hybrid option is now available for the devsim.interface_equation() (page 66) command. Please see Interface equation assembly (page 28) for information about boundary conditions.

2.7.5 Interface Equation Coupling

The name0, and name1 options are now available for the devsim.interface_equation() (page 66) command. They make it possible to couple dissimilar equation names across regions.

2.7.6 Interface and Contact Surface Area

Contact surface area is no longer included in SurfaceArea node model. It is now placed in ContactSurfaceArea. These are listed in Table 4.1.

2.7.7 Bug Fixes

- The devsim.interface_equation() (page 66) command is fixed for type=fluxterm boundary conditions on the interface.
- The devsim.get_material() (page 68), and devsim.set_material() (page 69) handle the contact option.
- Interface equation assembly skips nodes when an interface node is shared with a contact.

2.7.8 Extended Precision

The following new parameters are available:

- extended_solver, extended precision matrix for Newton and linear Solver
- extended_model, extended precision model evaluation
- extended_equation, extended precision equation assembly

When compiled with 128-bit extended precision support, these options enable calculations to be performed with higher precision. Default geometric models, are also calculated with extended precision.
Currently, the Linux and gcc-based Apple macOS versions have extended precision support.

2.8 May 15, 2017

2.8.1 Platforms

- The Ubuntu 16.04 (LTS) platform is now supported.
- The Ubuntu 12.04 (LTS), Centos 5 (Red Hat 5 compatible) platforms are no longer supported. These platforms are no longer supported by their vendors.
- Apple macOS compiled with flat_namespace to allow substitution of dynamically linked libraries.

2.8.2 Binary Releases

- Centos 6 released is linked against the Intel Math Kernel Library.
- Microsoft Windows 7 release is linked against the Intel Math Kernel Library
- Apple macOS can optionally use the Intel Math Kernel Library.
- Anaconda Python 2.7 is the recommended distribution.
- Please see release notes for more information.

2.8.3 Bug Fixes

- 3D element edge derivatives were not being evaluated correctly
- 3D equation model evaluation for element edge models

2.8.4 Enhancements

- Build scripts are provided to build on various platforms.
- DEVSIM mesh format stores elements, instead of just nodes, for contact and interfaces
- The devsim.create_gmsh_mesh() (page 74) command can be used to create a device from a provided list of elements.
2.8.5 Example Availability

- BJT simulation example available from https://github.com/devsim/devsim_bjt_example.

2.9 February 6, 2016

DEVSIM is now covered by the Apache License, Version 2.0 [ApacheSoftwareFoundation]. Please see the NOTICE and LICENSE file for more information.

2.10 November 24, 2015

2.10.1 Python Help

The Python interpreter now has documentation for each command, derived from the documentation in the manual. For example, help for the devsim.solve() (page 88) can be found using:

```
help("devsim.solve")
```

2.10.2 Manual Updates

The manual has been updated so that commands are easier to find in the index. Every command now has a short description. Cross references have been fixed. The date has been added to the front page.

2.11 November 1, 2015

2.11.1 Convergence Info

The devsim.solve() (page 88) now supports the info option. The solve command will then return convergence information.

2.11.2 Python Interpreter Changes

The way DEVSIM commands are loaded into the devsim module has been changed. It is now possible to see the full list of DEVSIM commands by typing

```
help('devsim')
```

in the Python interpreter.
2.11.3 Platform Improvements and Binary Availability

Many improvements have been made in the way binaries are generated for the Linux, Apple macOS, and Microsoft Windows platforms.

For Linux (see linux.txt):

- Create Centos 5, (Red Hat Enterprise Linux 5 compatible) build
- Build uses Intel Math Kernel Library math libraries (community edition)
- Build uses any compatible Python 2.7, including Anaconda
- Build compatible with newer Linux distributions.

For Apple macOS (see macos.txt):

- Uses the system Python 2.7 on macOS 10.10 (Yosemite)
- Provide instructions to use Anaconda Python

For Microsoft Windows (see windows.txt):

- Uses any compatible Python 2.7, including Anaconda
- Build uses Intel Math Kernel Library Community Edition

Binary releases are available for these platforms at https://devsim.org.

2.12 September 6, 2015

The `devsim.set_node_values()` (page 86) takes a new option, `values`. It is a list containing values to set for all of the nodes in a region.

The following new commands have been added:

- `devsim.get_equation_list()` (page 65)
- `devsim.get_contact_equation_list()` (page 65)
- `devsim.get_interface_equation_list()` (page 66)
- `devsim.delete_equation()` (page 64)
- `devsim.delete_contact_equation()` (page 63)
- `devsim.delete_interface_equation()` (page 64)
- `devsim.get_equation_command()` (page 65)
- `devsim.get_contact_equation_command()` (page 65)
- `devsim.get_interface_equation_command()` (page 66)
2.13 August 10, 2015

The `devsim.create_contact_from_interface()` (page 74) may be used to create a contact at the location of an interface. This is useful when contact boundary conditions are needed for a region connected to the interface.

2.14 July 16, 2015

The `devsim.set_node_value()` (page 86) was not properly setting the value. This issue is now resolved.

2.15 June 7, 2015

The `devsim.equation()` (page 64) now supports the `edge_volume_model`. This makes it possible to integrate edge quantities properly so that it is integrated with respect to the volume on nodes of the edge. To set the node volumes for integration, it is necessary to define a model for the node volumes on both nodes of the edge. For example:

```python
devsim.edge_model(device="device", region="region", name="EdgeNodeVolume",
equation="0.5*EdgeCouple*EdgeLength")
set_parameter(name="edge_node0_volume_model", value="EdgeNodeVolume")
set_parameter(name="edge_node1_volume_model", value="EdgeNodeVolume")
```

For the cylindrical coordinate system in 2D, please see *Cylindrical Coordinate Systems* (page 31).

macOS 10.10 (Yosemite) is now supported. Regression results in the source distribution are for a 2014 Macbook Pro i7 running this operating system.

2.16 October 4, 2014

2.16.1 Platform Availability

The software is now supported on the Microsoft Windows. Please see *Supported platforms* (page 55) for more information.

2.17 December 25, 2013

2.17.1 Binary Availability

Binary versions of the DEVSIM software are available for download from http://sourceforge.net/projects/devsim. Current versions available are for

- macOS 10.10 (Yosemite)
• Red Hat Enterprise Linux 6
• Ubuntu 12.04 (LTS)

Please see *Installation* (page 55) for more information.

**2.17.2 Platforms**

macOS 10.10 (Yosemite) is now supported. Support for 32 bit is no longer supported on this platform, since the operating system is only released as 64 bit.

Regression data will no longer be maintained in the source code repository for 32 bit versions of Ubuntu 12.04 (LTS) and Red Hat Enterprise Linux 6. Building and running on these platforms will still be supported.

**2.17.3 Source code improvements**

The source code has been improved to compile on macOS 10.10 (Yosemite) and to comply with C++11 language standards. Some of the structure of the project has been reorganized. These changes to the infrastructure will help to keep the program maintainable and useable into the future.

**2.18 September 8, 2013**

**2.18.1 Convergence**

If the simulation is diverging for 5 or more iterations, the simulation stops.

**2.18.2 Bernoulli Function Derivative Evaluation**

The \( \text{dBdx} \) math function has been improved to reduce overflow.

**2.18.3 Default Edge Model**

The edge_index is now a default edge models created on a region Table 4.2.

**2.19 August 14, 2013**

**2.19.1 SYMDIFF functions**

The vec_max and vec_min functions have been added to the SYMDIFF parser (Table 10.2). The vec_sum function replaces sum.
2.19.2 Default Node Models

The `coordinate_index` and `node_index` are now part of the default node models created on a region (Table 4.1).

2.19.3 Set Node Value

It is now possible to use the `devsim.set_node_value()` (page 86) to set a uniform value or indexed value on a node model.

2.19.4 Fix Edge Average Model

Fixed issue with `devsim.edge_average_model()` (page 78) during serialization to the DEVSIM format.

2.20 July 29, 2013

2.20.1 DEVSIM is open source

DEVSIM is now an open source project and is available from https://github.com/devsim/devsim. License information may be found in DEVSIM License (page 57). If you would like to participate in this project or need support, please contact us using the information in Contact (page 1). Installation instructions may be found in Installation (page 55).

2.20.2 Build

The Tcl interpreter version of DEVSIM is now called `devsim_tcl`, and is located in `/src/main/` of the build directory. Please see the INSTALL file for more information.

2.20.3 Contact Material

Contacts now require a material setting (e.g. metal). This is for informational purposes. Contact models still look up parameter values based on the region they are located.

2.20.4 External Meshing

Please see Using an external mesher (page 39) for more information about importing meshes from other tools.

Genius Mesh Import DEVSIM can now read meshes written from Genius Device Simulator. More information about Genius is in Genius (page 39).

Gmsh Mesh Import DEVSIM reads version 2.1 and 2.2 meshes from Gmsh. Version 2.0 is no longer supported. Please see Gmsh (page 40) for more information.
2.20.5 Math Functions

The acosh, asinh, atanh, are now available math functions. Please see Table 10.2.

2.20.6 Test directory structure

Platform specific results are stored in a hierarchical fashion.
Chapter 3

Introduction

3.1 Overview

**DEVSIM** is a technology computer-aided design (TCAD) software for semiconductor device simulation. While geared toward this application, it may be used where the control volume approach is appropriate for solving systems of partial-differential equations (PDE’s) on a static mesh. After introducing **DEVSIM**, the rest of the manual discusses the key components of the system, and instructions for their use.

**DEVSIM** is available from https://devsim.org. The source code is available under the terms of the Apache License Version 2.0 [ApacheSoftwareFoundation]. Examples are released under the Apache License Version 2.0 [ApacheSoftwareFoundation]. Contributions to this project are welcome in the form of bug reporting, documentation, modeling, and feature implementation.

3.2 Goals

The primary goal of **DEVSIM** is to give the user as much flexibility and control as possible. In this regard, few models are coded into the program binary. They are implemented in human-readable scripts that can be modified if necessary.

**DEVSIM** has a scripting language interface (**User Interface** (page 43)). This provides control structures and language syntax in a consistent and intuitive manner. The user is provided an environment where they can implement new models on their own. This is without requiring extensive vendor support or use of compiled programming languages.

**SYMDIFF** (**SYMDIFF** (page 47)) is the symbolic expression parser used to allow the formulation of device equations in terms of models and parameters. Using symbolic differentiation, the required partial derivatives can be generated, or provided by the user. **DEVSIM** then assembles these equations over the mesh.

3.3 Structures

**Devices** A device refers to a discrete structure being simulated. It is composed of the following types of objects.
**Regions** A region defines a portion of the device of a specific material. Each region has its own system of equations being solved.

**Interfaces** An interface connects two regions together. At the interfaces, equations are specified to account for how the flux in each device region crosses the region boundary.

**Contacts** A contact specifies the boundary conditions required for device simulation. It also specifies how terminal currents are integrated into an external circuit.

### 3.4 Equation assembly

Equation assembly of models is discussed in *Equation and Models* (page 19).

### 3.5 Parameters

Parameters may be specified globally, or for a specific device or region. Alternatively, parameters may be based on the material type of the regions. Usage is discussed in *Parameters* (page 33).

### 3.6 Circuits

Circuit boundary conditions allow multi-device simulation. They are also required for setting sources and their response for AC and noise analysis. Circuit elements, such as voltage sources, current sources, resistors, capacitors, and inductors may be specified. This is further discussed in *Circuits* (page 35).

### 3.7 Meshing

Meshing is discussed in *Meshing* (page 37).

### 3.8 Analysis

DEVSIM offers a range of simulation algorithms. They are discussed in more detail in *Solver* (page 41).

**DC** The DC operating point analysis is useful for performing steady-state simulation for a different bias conditions.

**AC** At each DC operating point, a small-signal AC analysis may be performed. An AC source is provided through a circuit and the response is then simulated. This is useful for both quasi-static capacitance simulation, as well as RF simulation.

**Noise/Sensitivity** Noise analysis may be used to evaluate how internal noise sources are observed in the terminal currents of the device or circuit. Using this method, it is also possible to simulate how the device response changes when device parameters are changed.
Transient DEVSIM is able to simulate the nonlinear transient behavior of devices, when the bias conditions change with time.

### 3.9 Scripting interface

The scripting interface to DEVSIM is discussed in *User Interface* (page 43).

### 3.10 Expression parser

The expression parser is discussed in *SYMDIFF* (page 47).

### 3.11 Visualization and postprocessing

Visualization is discussed in *Visualization* (page 53).

### 3.12 Installation

Installation is discussed in *Installation* (page 55).

### 3.13 Additional information

Additional information is discussed in *Additional Information* (page 57).

### 3.14 Examples

Examples are discussed in the remaining chapters beginning with *Example Overview* (page 91).
Chapter 4

Equation and Models

4.1 Overview

DEVSIM uses the control volume approach for assembling partial-differential equations (PDE’s) on the simulation mesh. DEVSIM is used to solve equations of the form:

$$\frac{\partial X}{\partial t} + \nabla \cdot \vec{Y} + Z = 0$$

Internally, it transforms the PDE’s into an integral form.

$$\int \frac{\partial X}{\partial t} \, dr + \int \vec{Y} \cdot \partial s + \int Z \, dr = 0$$

Equations involving the divergence operators are converted into surface integrals, while other components are integrated over the device volume.

In Fig. 4.1, 2D mesh elements are depicted. The shaded area around the center node is referred to as the node volume, and it is used for the volume integration. The lines from the center node to other nodes are referred to as edges. The flux through the edge are integrated with respect to the perpendicular bisectors (dashed lines) crossing each triangle edge.

In this form, we refer to a model integrated over the edges of triangles as edge models. Models integrated over the volume of each triangle vertex are referred to as node models. Element edge models are a special case where variables at other nodes off the edge may cause the flux to change.

There are a default set of models created in each region upon initialization of a device, and are typically based on the geometrical attributes. These are described in the following sections. Models required for describing the device behavior are created using the equation parser described in SYMDIFF (page 47). For special situations, custom matrix assembly is also available and is discussed in Custom matrix assembly (page 30).
Fig. 4.1: Mesh elements in 2D.
Fig. 4.2: Edge model constructs in 2D.
Fig. 4.3: Element edge model constructs in 2D.
4.2 Bulk models

4.2.1 Node models

Node models may be specified in terms of other node models, mathematical functions, and parameters on the device. The simplest model is the node solution, and it represents the solution variables being solved for. Node models automatically created for a region are listed in Table 4.1.

In this example, we present an implementation of Shockley Read Hall recombination [MKC02].

```python
USRH="-ElectronCharge*(Electrons*Holes - n_i^2)/(taup*(Electrons + n1) \\
+ taun*(Holes + p1))"

dUSRHdn="simplify(diff(%s, Electrons))" % USRH
dUSRHdp="simplify(diff(%s, Holes))" % USRH
devsim.node_model(device='MyDevice', region='MyRegion',
            name="USRH", equation=USRH)
devsim.node_model(device='MyDevice', region='MyRegion',
            name="USRH:Electrons", equation=dUSRHdn)
devsim.node_model(device='MyDevice', region='MyRegion',
            name="USRH:Holes", equation=dUSRHdp)
```

The first model specified, USRH, is the recombination model itself. The derivatives with respect to electrons and holes are USRH:Electrons and USRH:Holes, respectively. In this particular example Electrons and Holes have already been defined as solution variables. The remaining variables in the equation have already been specified as parameters.

The `diff` function tells the equation parser to take the derivative of the original expression, with respect to the variable specified as the second argument. During equation assembly, these derivatives are required in order to converge upon a solution. The `simplify` function tells the expression parser to attempt to simplify the expression as much as possible.

Table 4.1: Node models defined on each region of a device.

<table>
<thead>
<tr>
<th>Node Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>AtContactNode</td>
<td>Evaluates to 1 if node is a contact node, otherwise 0</td>
</tr>
<tr>
<td>NodeVolume</td>
<td>The volume of the node. Used for volume integration of node models on nodes in mesh</td>
</tr>
<tr>
<td>NSurfaceNormal_x</td>
<td>The surface normal to points on the interface or contact (2D and 3D)</td>
</tr>
<tr>
<td>NSurfaceNormal_y</td>
<td>The surface normal to points on the interface or contact (2D and 3D)</td>
</tr>
<tr>
<td>NSurfaceNormal_z</td>
<td>The surface normal to points on the interface or contact (3D)</td>
</tr>
<tr>
<td>SurfaceArea</td>
<td>The surface area of a node on interface nodes, otherwise 0</td>
</tr>
<tr>
<td>ContactSurfaceArea</td>
<td>The surface area of a node on contact nodes, otherwise 0</td>
</tr>
<tr>
<td>coordinate_index</td>
<td>Coordinate index of the node on the device</td>
</tr>
<tr>
<td>node_index</td>
<td>Index of the node in the region</td>
</tr>
<tr>
<td>x</td>
<td>x position of the node</td>
</tr>
<tr>
<td>y</td>
<td>y position of the node</td>
</tr>
<tr>
<td>z</td>
<td>z position of the node</td>
</tr>
</tbody>
</table>
4.2.2 Edge models

Edge models may be specified in terms of other edge models, mathematical functions, and parameters on the device. In addition, edge models may reference node models defined on the ends of the edge. As depicted in Fig. 4.2, edge models are with respect to the two nodes on the edge, n0 and n1.

For example, to calculate the electric field on the edges in the region, the following scheme is employed:

```python
devsim.edge_model(device="device", region="region", name="ElectricField",
                   equation="(Potential@n0 - Potential@n1)*EdgeInverseLength")
devsim.edge_model(device="device", region="region",
                   name="ElectricField:Potential@n0", equation="EdgeInverseLength")
devsim.edge_model(device="device", region="region",
                   name="ElectricField:Potential@n1", equation="-EdgeInverseLength")
```

In this example, `EdgeInverseLength` is a built-in model for the inverse length between nodes on an edge. `Potential@n0` and `Potential@n1` is the `Potential` node solution on the nodes at the end of the edge. These edge quantities are created using the `devsim.edge_from_node_model()` (page 79). In addition, the `devsim.edge_average_model()` (page 78) can be used to create edge models in terms of node model quantities.

Edge models automatically created for a region are listed in Table 4.2.

<table>
<thead>
<tr>
<th>Edge Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EdgeCouple</td>
<td>The length of the perpendicular bisector of an element edge. Used to perform surface integration of edge models on edges in mesh.</td>
</tr>
<tr>
<td>EdgeInverseLength</td>
<td>Inverse of the EdgeLength.</td>
</tr>
<tr>
<td>EdgeLength</td>
<td>The distance between the two nodes of an edge</td>
</tr>
<tr>
<td>edge_index</td>
<td>Index of the edge on the region</td>
</tr>
<tr>
<td>unitx</td>
<td>x component of the unit vector along an edge</td>
</tr>
<tr>
<td>unity</td>
<td>y component of the unit vector along an edge (2D and 3D)</td>
</tr>
<tr>
<td>unitz</td>
<td>z component of the unit vector along an edge (3D only)</td>
</tr>
</tbody>
</table>

4.2.3 Element edge models

Element edge models are used when the edge quantities cannot be specified entirely in terms of the quantities on both nodes of the edge, such as when the carrier mobility is dependent on the normal electric field. In 2D, element edge models are evaluated on each triangle edge. As depicted in Fig. 4.3, edge models are with respect to the three nodes on each triangle edge and are denoted as en0, en1, and en2. Derivatives are with respect to each node on the triangle.

In 3D, element edge models are evaluated on each tetrahedron edge. Derivatives are with respect to the nodes on both triangles on the tetrahedron edge. Element edge models automatically created for a region are listed in Table 4.3.

As an alternative to treating integrating the element edge model with respect to `ElementEdgeCouple`, the integration may be performed with respect to `ElementNodeVolume`. See `devsim.equation()` (page 64) for more information.
**Table 4.3: Element edge models defined on each region of a device.**

<table>
<thead>
<tr>
<th>Element Edge Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ElementEdgeCouple</td>
<td>The length of the perpendicular bisector of an edge. Used to perform</td>
</tr>
<tr>
<td></td>
<td>surface integration of element edge model on element edge in the mesh.</td>
</tr>
<tr>
<td>ElementNodeVolume</td>
<td>The node volume at either end of each element edge.</td>
</tr>
</tbody>
</table>

### 4.2.4 Model derivatives

To converge upon the solution, derivatives are required with respect to each of the solution variables in the system. **DEVSIM** will look for the required derivatives. For a model `model`, the derivatives with respect to solution variable `variable` are presented in **Table 4.4**.

**Table 4.4: Required derivatives for equation assembly.** `model` is the name of the model being evaluated, and `variable` is one of the solution variables being solved at each node.

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Derivatives Required</th>
</tr>
</thead>
<tbody>
<tr>
<td>Node Model</td>
<td><code>model:variable</code></td>
</tr>
<tr>
<td>Edge Model</td>
<td><code>model:variable@n0, model:variable@n1</code></td>
</tr>
<tr>
<td>Element Edge Model</td>
<td><code>model:variable@en0, model:variable@en1, model:variable@en2, model:variable@en3 (3D)</code></td>
</tr>
</tbody>
</table>

### 4.2.5 Conversions between model types

The `devsim.edge_from_node_model()` (page 79) is used to create edge models referring to the nodes connecting the edge. For example, the edge models `Potential@n0` and `Potential@n1` refer to the `Potential` node model on each end of the edge.

The `devsim.edge_average_model()` (page 78) creates an edge model which is either the arithmetic mean, geometric mean, gradient, or negative of the gradient of the node model on each edge.

When an edge model is referred to in an element edge model expression, the edge values are implicitly converted into element edge values during expression evaluation. In addition, derivatives of the edge model with respect to the nodes of an element edge are required, they are converted as well. For example, `edgemodel:variable@n0` and `edgemodel:variable@n1` are implicitly converted to `edgemodel:variable@en0` and `edgemodel:variable@en1`, respectively.

The `devsim.element_from_edge_model()` (page 80) is used to create directional components of an edge model over an entire element. The derivative option is used with this command to create the derivatives with respect to a specific node model. The `devsim.element_from_node_model()` (page 81) is used to create element edge models referring to each node on the element of the element edge.

### 4.2. Bulk models

---

25
4.2.6 Equation assembly

Bulk equations are specified in terms of the node, edge, and element edge models using the `devsim.equation()` (page 64). Node models are integrated with respect to the node volume. Edge models are integrated with the perpendicular bisectors along the edge onto the nodes on either end.

Element edge models are treated as flux terms and are integrated with respect to `ElementEdgeCouple` using the `element_model` option. Alternatively, they may be treated as source terms and are integrated with respect to `ElementNodeVolume` using the `volume_model` option.

In this example, we are specifying the Potential Equation in the region to consist of a flux term named `PotentialEdgeFlux` and to not have any node volume terms.

```python
devsim.equation(device="device", region="region", name="PotentialEquation", variable_name="Potential", edge_model="PotentialEdgeFlux", variable_update="log_damp" )
```

In addition, the solution variable coupled with this equation is `Potential` and it will be updated using logarithmic damping.

Table 4.5: Required derivatives for interface equation assembly. The node model name `nodemodel` and its derivatives `nodemodel:variable` are suffixed with `@r0` and `@r1` to denote which region on the interface is being referred to.

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Model Name</th>
<th>Derivatives Required</th>
</tr>
</thead>
<tbody>
<tr>
<td>Node Model (region 0)</td>
<td>nodemodel@r0</td>
<td>nodemodel:variable@r0</td>
</tr>
<tr>
<td>Node Model (region 1)</td>
<td>nodemodel@r1</td>
<td>nodemodel:variable@r1</td>
</tr>
<tr>
<td>Interface Node Model</td>
<td>inodemodel</td>
<td>inodemodel:variable@r0,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>inodemodel:variable@r1</td>
</tr>
</tbody>
</table>

4.3 Interface

4.3.1 Interface models

Fig. 4.4 depicts an interface in `DEVSIM`. It is a collection of overlapping nodes existing in two regions, `r0` and `r1`.

Interface models are node models specific to the interface being considered. They are unique from bulk node models, in the sense that they may refer to node models on both sides of the interface. They are specified using the `devsim.interface_model()` (page 84). Interface models may refer to node models or parameters on either side of the interface using the syntax `nodemodel@r0` and `nodemodel@r1` to refer to the node model in the first and second regions of the interface. The naming convention for node models, interface node models, and their derivatives are shown in Table 4.5.

```python
devsim.interface_model(device="device", interface="interface", name="continuousPotential", equation="Potential@r0-Potential@r1")
```
Fig. 4.4: Interface constructs in 2D. Interface node pairs are located at each ●. The SurfaceArea model is used to integrate flux term models.
4.3.2 Interface model derivatives

For a given interface model, `model`, the derivatives with respect to the variable `variable` in the regions are

- `model:variable@r0`
- `model:variable@r1`

```python
devsim.interface_model(device="device", interface="interface", name="continuousPotential:Potential@r0", equation="1")
devsim.interface_model(device="device", interface="interface", name="continuousPotential:Potential@r1", equation="-1")
```

4.3.3 Interface equation assembly

There are three types of interface equations considered in DEVSIM. They are both activated using the `devsim.interface_equation()` (page 66).

In the first form, `continuous`, the equations for the nodes on both sides of the interface are integrated with respect to their volumes and added into the same equation. An additional equation is then specified to relate the variables on both sides. In this example, continuity in the potential solution across the interface is enforced, using the `continuousPotential` model defined in the previous section.

```python
devsim.interface_equation(device="device", interface="interface", name=...
    variable_name="Potential", interface_model="continuousPotential",
    type="continuous")
```

In the second form, `fluxterm`, a flux term is integrated over the surface area of the interface and added to the first region, and subtracted from the second.

In the third form, `hybrid`, equations for nodes on both sides of the interface are added into the equation for the node in the first region. The equation for the node on the second interface is integrated in the second region, and the fluxterm is subtracted in the second region.

4.4 Contact

4.4.1 Contact models

Fig. 4.5 depicts how a contact is treated in a simulation. It is a collection of nodes on a region. During assembly, the specified models form an equation, which replaces the equation applied to these nodes for a bulk node.

Contact models are equivalent to node and edge models, and are specified using the `devsim.contact_node_model()` (page 76) and the `devsim.contact_edge_model()` (page 76), respectively. The key difference is that the models are only evaluated on the contact nodes for the contact specified.
4.4.2 Contact model derivatives

The derivatives are equivalent to the discussion in Model derivatives (page 25). If external circuit boundary conditions are being used, the model derivative with respect to the circuit node name should be specified as model:node.

4.4.3 Contact equation assembly

The devsim.contact_equation() (page 62) is used to specify the boundary conditions on the contact nodes. The models specified replace the models specified for bulk equations of the same name. For example, the node model specified for the contact equation is assembled on the contact nodes, instead of the node model specified for the bulk equation. Contact equation models not specified are not assembled, even if the model exists on the bulk equation for the region attached to the contact.

As an example

```python
devsim.contact_equation(device="device", contact="contact", name="PotentialEquation", variable_name="Potential", node_model="contact_bc", edge_charge_model="DField")
```

Current models refer to the instantaneous current flowing into the device. Charge models refer to the instantaneous charge at the contact.

During a transient, small-signal or ac simulation, the time derivative is taken so that the net current into a
circuit node is

\[ I(t) = i(t) + \frac{\partial q(t)}{\partial t} \]

where \( i \) is the integrated current and \( q \) is the integrated charge.

### 4.5 Custom matrix assembly

The `devsim.custom_equation()` (page 63) command is used to register callbacks to be called during matrix and right hand side assembly. The Python procedure must expect to receive two arguments and return two lists. For example a procedure named `myassemble` registered with

```python
devsim.custom_equation(name="test1", procedure="myassemble")
```

must expect to receive two arguments

```python
def myassemble(what, timemode):
    .
    .
    return [rcv, rv]
```

where `what` may be passed as one of

- `MATRIXONLY`
- `RHS`
- `MATRIXANDRHS`

and `timemode` may be passed as one of

- `DC`
- `TIME`

When `timemode` is `DC`, the time-independent part of the equation is returned. When `timemode` is `TIME`, the time-derivative part of the equation is returned. The simulator will scale the time-derivative terms with the proper frequency or time scale.

The return value from the procedure must return two lists of the form

\[
\begin{bmatrix}
1 & 1 & 1.0 & 2 & 2 & 1.0 & 2 & 2 & 1.0 & 2 & 2 & 1.0 & 1.0 & 2 & 1 & 2 & 1.0 & 2 & 1 & 2 & -1.0 & 2 & 2 & 1.0 & 1.0 & 2 & 1 & 2 & 1.0 & 2 & 1 & 2 & -1.0
\end{bmatrix}
\]

where the length of the first list is divisible by 3 and contains the row, column, and value to be assembled into the matrix. The second list is divisible by 2 and contains the right-hand side entries. Either list may be empty.

The `devsim.get_circuit_equation_number()` (page 62) may be used to get the equation numbers corresponding to circuit node names. The `devsim.get_equation_numbers()` (page 65) may be used to find the equation number corresponding to each node index in a region.

The matrix and right hand side entries should be scaled by the `NodeVolume` if they are assembled into locations in a device region. Row permutations, required for contact and interface boundary conditions, are automatically applied to the row numbers returned by the Python procedure.
4.6 Cylindrical Coordinate Systems

In 2D, models representing the edge couples, surface areas and node volumes may be generated using the following commands:

- `devsim.cylindrical_edge_couple()` (page 76)
- `devsim.cylindrical_node_volume()` (page 77)
- `devsim.cylindrical_surface_area()` (page 77)

In order to change the integration from the default models to cylindrical models, the following parameters may be set

```python
set_parameter(name="node_volume_model", value="CylindricalNodeVolume")
set_parameter(name="edge_couple_model", value="CylindricalEdgeCouple")
set_parameter(name="edge_node0_volume_model", value="CylindricalEdgeNodeVolume@n0")
set_parameter(name="edge_node1_volume_model", value="CylindricalEdgeNodeVolume@n1")
set_parameter(name="element_edge_couple_model", value="ElementCylindricalEdgeCouple")
set_parameter(name="element_node0_volume_model", value="ElementCylindricalNodeVolume@en0")
set_parameter(name="element_node1_volume_model", value="ElementCylindricalNodeVolume@en1")
```
Chapter 5

Parameters

Parameters can be set using the commands in *Material Commands* (page 67). There are two complementary formalisms for doing this.

5.1 Parameters

Parameters are set globally, on devices, or on regions of a device. The models on each device region are automatically updated whenever parameters change.

```python
devsim.set_parameter(device="device", region="region",
                     name="ThermalVoltage", value=0.0259)
```

They may also be used to control program behavior, as listed in *Table 5.1*:
Table 5.1: Parameters controlling program behavior.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>debug_level</td>
<td>info, verbose Section 9.3.5</td>
</tr>
<tr>
<td>threads_available</td>
<td>value=1, Section 9.3.6</td>
</tr>
<tr>
<td>threads_task_size</td>
<td>value=?, Section 9.3.6</td>
</tr>
<tr>
<td>node_volume_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>edge_couple_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>edge_node0_volume_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>edge_node1_volume_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>element_edge_couple_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>element_node0_volume_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>element_node1_volume_model</td>
<td>Section 4.6</td>
</tr>
<tr>
<td>extended_solver</td>
<td>value=False Extended precision matrix and RHS assembly and error evaluations. Linear solver and circuit assembly is still double precision’’</td>
</tr>
<tr>
<td>extended_model</td>
<td>value=False Extended precision model evaluation</td>
</tr>
<tr>
<td>extended_equation</td>
<td>value=False Extended precision equation evaluation</td>
</tr>
</tbody>
</table>

5.2 Material database entries

Alternatively, parameters may be set based on material types. A database file is used for getting values on the regions of the device.

```python
devsim.create_db(filename="foodb")
devsim.add_db_entry(material="global", parameter="q", value=1.60217646e-19, unit="coul", description="Electron Charge")
devsim.add_db_entry(material="Si", parameter="one", value=1, unit="", description="")
devsim.close_db
```

When a database entry is not available for a specific material, the parameter will be looked up on the global material entry.

5.3 Discussion

Both parameters and material database entries may be used in model expressions. Parameters have precedence in this situation. If a parameter is not found, then DEVSIM will also look for a circuit node by the name used in the model expression.
Chapter 6

Circuits

6.1 Circuit elements

Circuit elements are manipulated using the commands in *Circuit Commands* (page 61). Using the `devsim.circuit_element()` (page 61) to add a circuit element will implicitly create the nodes being references.

A simple resistor divider with a voltage source would be specified as:

```python
devsim.circuit_element(name="V1", n1="1", n2="0", value=1.0)
devsim.circuit_element(name="R1", n1="1", n2="2", value=5.0)
devsim.circuit_element(name="R2", n1="2", n2="0", value=5.0)
```

Circuit nodes are created automatically when referred to by these commands. Voltage sources create an additional circuit node of the form `V1.I` to account for the current flowing through it.

6.2 Connecting devices

For devices to contribute current to an external circuit, the `devsim.contact_equation()` (page 62) should use the `circuitnode` option to specify the circuit node in which to integrate its current. This option does not create a node in the circuit. No circuit boundary condition for the contact equation will exist if the circuit node does not actually exist in the circuit. The `devsim.circuit_node_alias()` (page 62) may be used to associate the name specified on the contact equation to an existing circuit node on the circuit.

The circuit node names may be used in any model expression on the regions and interfaces. However, the simulator will only take derivatives with respect to circuit nodes names on models used to compose the contact equation.
Chapter 7

Meshing

7.1 1D meshing

DEVSIM has an internal 1D mesher and the proper sequence of commands follow in this example.

```python
devsim.create_1d_mesh(mesh="cap")
devsim.add_1d_mesh_line(mesh="cap", pos=0, ps=0.1, tag="top")
devsim.add_1d_mesh_line(mesh="cap", pos=0.5, ps=0.1, tag="mid")
devsim.add_1d_mesh_line(mesh="cap", pos=1, ps=0.1, tag="bot")
devsim.add_1d_contact(mesh="cap", name="top", tag="top", material="metal")
devsim.add_1d_contact(mesh="cap", name="bot", tag="bot", material="metal")
devsim.add_1d_interface(mesh="cap", name="MySiOx", tag="mid")
devsim.add_1d_region(mesh="cap", material="Si", region="MySiRegion", tag1="top", tag2="mid")
devsim.add_1d_region(mesh="cap", material="Ox", region="MyOxRegion", tag1="mid", tag2="bot")
devsim.finalize_mesh(mesh="cap")
devsim.create_device(mesh="cap", device="device")
```

The `devsim.create_1d_mesh()` (page 73) is first used to initialize the specification of a new mesh by the name specified with the `mesh` option. The `devsim.add_1d_mesh_line()` (page 70) is used to specify the end points of the 1D structure, as well as the location of points where the spacing changes. The command is used to create reference labels used for specifying the contacts, interfaces and regions.

The `devsim.add_1d_contact()` (page 70), `devsim.add_1d_interface()` (page 70) and `devsim.add_1d_region()` (page 70) are used to specify the contacts, interfaces and regions for the device.

Once the meshing commands have been completed, the `devsim.finalize_mesh()` (page 75) is called to create a mesh structure and then `devsim.create_device()` (page 74) is used to create a device using the mesh.
7.2 2D mesher

Similar to the 1D mesher, the 2D mesher uses a sequence of non-terminating mesh lines are specified in both the x and y directions to specify a mesh structure. As opposed to using tags, the regions are specified using `devsim.add_2d_region()` (page 72) as box coordinates on the mesh coordinates. The contacts and interfaces are specified using boxes, however it is best to ensure the the interfaces and contacts encompass only one line of points.

```python
devsim.create_2d_mesh(mesh="cap")
devsim.add_2d_mesh_line(mesh="cap", dir="y", pos=-0.001, ps=0.001)
devsim.add_2d_mesh_line(mesh="cap", dir="x", pos=xmin, ps=0.1)
devsim.add_2d_mesh_line(mesh="cap", dir="x", pos=xmax, ps=0.1)
devsim.add_2d_mesh_line(mesh="cap", dir="y", pos=ymin, ps=0.1)
devsim.add_2d_mesh_line(mesh="cap", dir="y", pos=+1.001, ps=0.001)
devsim.add_2d_region(mesh="cap", material="gas", region="gas1", yl=-.001, yh=0.0)
devsim.add_2d_region(mesh="cap", material="gas", region="gas2", yl=1.0, yh=1.001)
devsim.add_2d_region(mesh="cap", material="Oxide", region="r0", xl=xmin, xh=xmax, yl=ymid1, yh=ymin)
devsim.add_2d_region(mesh="cap", material="Silicon", region="r1", xl=xmin, xh=xmax, yl=ymid2, yh=ymid1)
devsim.add_2d_region(mesh="cap", material="Silicon", region="r2", xl=xmin, xh=xmax, yl=ymid2, yh=ymax)
devsim.add_2d_interface(mesh="cap", name="i0", region0="r0", region1="r1")
devsim.add_2d_interface(mesh="cap", name="i1", region0="r1", region1="r2", xl=0, xh=1, yl=ymid2, yh=ymid2, bloat=1.0e-10)
devsim.add_2d_contact(mesh="cap", name="top", region="r0", yl=ymin, yh=ymin, bloat=1.0e-10, material="metal")
devsim.add_2d_contact(mesh="cap", name="bot", region="r2", yl=ymax, yh=ymax, bloat=1.0e-10, material="metal")
devsim.finalize_mesh(mesh="cap")
devsim.create_device(mesh="cap", device="device")
```

In the current implementation of the software, it is necessary to create a region on both sides of the contact in order to create a contact using `devsim.add_2d_contact()` (page 71) or an interface using `devsim.add_2d_interface()` (page 71).

Once the meshing commands have been completed, the `devsim.finalize_mesh()` (page 75) is called to create a mesh structure and then `devsim.create_device()` (page 74) is used to create a device using the mesh.
7.3 Using an external mesher

DEVSIM supports reading meshes from Gmsh. Support for Genius Device Simulator is deprecated and will be removed from a future release. In addition, meshes may be input directly using the Python interface. These meshes may only contain points, lines, triangles, and tetrahedra. Hybrid meshes or uniform meshes containing other elements are not supported at this time.

7.3.1 Genius

Meshes from the Genius Device Simulator software (see Genius (page 57)) can be imported using the CGNS format. In this example, devsim.create_genius_mesh() (page 74) returns region and boundary information which can be used to setup the device.

```python
mesh_name = "nmos_iv"
result = create_genius_mesh(file="nmos_iv.cgns", mesh=mesh_name)

contacts = {}
for region_name, region_info in result['mesh_info']['regions'].iteritems():
    add_genius_region(mesh=mesh_name, genius_name=region_name, region=region_name, material=region_info['material'])
    for boundary, is_electrode in region_info['boundary_info'].iteritems():
        if is_electrode:
            if boundary in contacts:
                contacts[boundary].append(region_name)
            else:
                contacts[boundary] = [region_name, ]
        else:
            contacts[boundary] = [region_name, ]

for contact, regions in contacts.iteritems():
    if len(regions) == 1:
        add_genius_contact(mesh=mesh_name, genius_name=contact, name=contact, region=regions[0], material='metal')
    else:
        for region in regions:
            add_genius_contact(mesh=mesh_name, genius_name=contact, name=contact+'@'+region, region=region, material='metal')

for boundary_name, regions in result['mesh_info']['boundaries'].iteritems():
    if len(regions) == 2:
        add_genius_interface(mesh=mesh_name, genius_name=boundary_name, name=boundary_name, region0=regions[0], region1=regions[1])

finalize_mesh(mesh=mesh_name)
create_device(mesh=mesh_name)
```

Example locations are available on genius (page 91).
7.3.2 Gmsh

The Gmsh meshing software (see Gmsh (page 57)) can be used to create a 1D, 2D, or 3D mesh suitable for use in DEVSIM. When creating the mesh file using the software, use physical group names to map the difference entities in the resulting mesh file to a group name. In this example, a MOS structure is read in:

```python
devsim.create_gmsh_mesh(file="gmsh_mos2d.msh", mesh="mos2d")
devsim.add_gmsh_region(mesh="mos2d" gmsh_name="bulk", region="bulk", material="Silicon")
devsim.add_gmsh_region(mesh="mos2d" gmsh_name="oxide", region="oxide", material="Silicon")
devsim.add_gmsh_region(mesh="mos2d" gmsh_name="gate", region="gate", material="Silicon")
devsim.add_gmsh_contact(mesh="mos2d" gmsh_name="drain_contact", region="bulk", name="drain", material="metal")
devsim.add_gmsh_contact(mesh="mos2d" gmsh_name="source_contact", region="bulk", name="source", material="metal")
devsim.add_gmsh_contact(mesh="mos2d" gmsh_name="body_contact", region="bulk", name="body", material="metal")
devsim.add_gmsh_contact(mesh="mos2d" gmsh_name="gate_contact", region="gate", name="gate", material="metal")
devsim.add_gmsh_interface(mesh="mos2d" gmsh_name="gate_oxide_interface", region0="gate", region1="oxide", name="gate_oxide")
devsim.add_gmsh_interface(mesh="mos2d" gmsh_name="bulk_oxide_interface", region0="bulk", region1="oxide", name="bulk_oxide")
devsim.finalize_mesh(mesh="mos2d")
devsim.create_device(mesh="mos2d", device="mos2d")
```

Once the meshing commands have been completed, the `devsim.finalize_mesh()` (page 75) is called to create a mesh structure and then `devsim.create_device()` (page 74) is used to create a device using the mesh.

7.3.3 Custom mesh loading using scripting

It is also possible to arbitrarily load a mesh from a Python using the `devsim.create_gmsh_mesh()` (page 74). This is explained in the Notes section of the command.

7.4 Loading and saving results

The `devsim.write_devices()` (page 75) is used to create an ASCII file suitable for saving data for restarting the simulation later. The `devsim` format encodes structural information, as well as the commands necessary for generating the models and equations used in the simulation. The `devsim_data` format is used for storing numerical information for use in other programs for analysis. The `devsim.load_devices()` (page 75) is then used to reload the device data for restarting the simulation.
Chapter 8

Solver

8.1 Solver

DEVSIM uses Newton methods to solve the system of PDE’s. All of the analyses are performed using the `devsim.solve()` (page 88).

8.2 DC analysis

A DC analysis is performed using the `devsim.solve()` (page 88).

```
solve(type="dc", absolute_error=1.0e10, relative_error=1e-7, maximum_iterations=30)
```

8.3 AC analysis

An AC analysis is performed using the `devsim.solve()` (page 88). A circuit voltage source is required to set the AC source.

8.4 Noise/Sensitivity analysis

An noise analysis is performed using the `devsim.solve()` (page 88) command. A circuit node is specified in order to find its sensitivity to changes in the bulk quantities of each device. If the circuit node is named `V1.I`. A noise simulation is performed using:

```
solve(type="noise", frequency=1e5, output_node="V1.I")
```

Noise and sensitivity analysis is performed using the `devsim.solve()` (page 88). If the equation begins solved is `PotentialEquation`, the names of the scalar impedance field is then:

- `V1.I_PotentialEquation_real`
• \texttt{V1.I\_PotentialEquation\_imag}

and the vector impedance fields evaluated on the nodes are

• \texttt{V1.I\_PotentialEquation\_real\_gradx}
• \texttt{V1.I\_PotentialEquation\_imag\_gradx}
• \texttt{V1.I\_PotentialEquation\_real\_grady} (2D and 3D)
• \texttt{V1.I\_PotentialEquation\_imag\_grady} (2D and 3D)
• \texttt{V1.I\_PotentialEquation\_real\_gradz} (3D only)
• \texttt{V1.I\_PotentialEquation\_imag\_gradz} (3D only)

### 8.5 Transient analysis

Transient analysis is performed using the \texttt{devsim.solve()} (page 88). DEVSIM supports time-integration of the device PDE’s. The three methods are supported are:

• BDF1
• TRBDF
• BDF2
Chapter 9

User Interface

9.1 Starting DEVSIM

Refer to Installation (page 55) for instructions on how to install DEVSIM. Once installed, DEVSIM may be invoked using the following command:

By first setting the PYTHONPATH variable to the lib directory in the DEVSIM distribution, devsim is loaded by using:

```python
import devsim
```

from Python.

Many of the examples in the distribution rely on the python_packages module, which is available by using:

```python
import devsim.python_packages
```

The default version of Python for use in scripts is 3.7, however scripts written for earlier versions of Python 3 should work. Python 2.7 is deprecated for future development.

9.2 Python Language

9.2.1 Introduction

Python is the scripting language employed as the text interface to DEVSIM. Documentation and tutorials for the language are available from [pyt]. A paper discussing the general benefits of using scripting languages may be found in [Ous98].

9.2.2 DEVSIM commands

All of commands are in the devsim namespace. In order to invoke a command, the command should be prefixed with devsim., or the following may be placed at the beginning of the script:
For details concerning error handling, please see Error handling (page 44).

9.2.3 Advanced usage

In this manual, more advanced usage of the Python language may be used. The reader is encouraged to use a suitable reference to clarify the proper use of the scripting language constructs, such as control structures.

9.2.4 Unicode Support

Internally, DEVSIM uses UTF-8 encoding, and expects model equations and saved mesh files to be written using this encoding. Users are encouraged to use the standard ASCII character set if they do not wish to use this feature. Python 3 interpreters handle UTF-8 encoding well. For the deprecated Python 2 interpreter, it is necessary to put the following line at the beginning of the python script.

```
# -*- coding: utf-8 -*-
```

On some systems, such as Microsoft Windows, it may be necessary to set the following environment variable before running a script containing UTF-8 characters.

```
SET PYTHONIOENCODING=utf-8
```

Care should be taken when using UTF-8 characters in names for visualization using the tools in Visualization (page 53), as this character set may not be supported.

9.3 Error handling

9.3.1 Python errors

When a syntax error occurs in a Python script an exception may be thrown. If it is uncaught, then DEVSIM will terminate. More details may be found in an appropriate reference. An exception that is thrown by DEVSIM is of the type devsim.error. It may be caught.

9.3.2 Fatal errors

When DEVSIM enters a state in which it may not recover. The interpreter should throw a Python exception with a message DEVSIM FATAL. At this point DEVSIM may enter an inconsistent state, so it is suggested not to attempt to continue script execution if this occurs.

In rare situations, the program may behave in an erratic manner, print a message, such as UNEXPECTED or terminate abruptly. Please report this using the contact information in Contact (page 1).
9.3.3 Floating point exceptions

During model evaluation, DEVSIM will attempt to detect floating point issues and return an error with some diagnostic information printed to the screen, such as the symbolic expression being evaluated. Floating point errors may be characterized as invalid, division by zero, and numerical overflow. This is considered to be a fatal error.

9.3.4 Solver errors

When using the `devsim.solve()` (page 88), the solver may not converge and a message will be printed and an exception may be thrown. The solution will be restored to its previous value before the simulation began. This exception may be caught and the bias conditions may be changed so the simulation may be continued. For example:

```python
try:
    solve(type="dc", absolute_error=abs_error,
          relative_error=rel_error, maximum_iterations=max_iter)
except devsim.error as msg:
    if msg[0].find("Convergence failure") != 0:
        raise
    ### put code to modify step here.
```

9.3.5 Verbosity

The `set_parameter()` may be used to set the verbosity globally, per device, or per region. Setting the `debug_level` parameter to `info` results in the default level of information to the screen. Setting this option to `verbose` or any other name results in more information to the screen which may be useful for debugging.

The following example sets the default level of debugging for the entire simulation, except that the gate region will have additional debugging information.

```python
devsim.set_parameter(name="debug_level", value="info")
devsim.set_parameter(device="device" region="gate",
                     name="debug_level", value="verbose")
```

9.3.6 Parallelization

Routines for the evaluating of models have been parallelized. In order to select the number of threads to use

```python
devsim.set_parameter(name="threads_available", value=2)
```

where the value specified is the number of threads to be used. By default, DEVSIM does not use threading. For regions with a small number of elements, the time for switching threads is more than the time to evaluate in a single thread. To set the minimum number of elements for a calculation, set the following parameter.
The Intel Math Kernel Library is parallelized, the number of thread may be controlled by setting the `MKL_NUM_THREADS` environment variable.
Chapter 10

SYMDIFF

10.1 Overview

SYMDIFF is a tool capable of evaluating derivatives of symbolic expressions. Using a natural syntax, it is possible to manipulate symbolic equations in order to aid derivation of equations for a variety of applications. It has been tailored for use within DEVSIM.

10.2 Syntax

10.2.1 Variables and numbers

Variables and numbers are the basic building blocks for expressions. A variable is defined as any sequence of characters beginning with a letter and followed by letters, integer digits, and the _ character. Note that the letters are case sensitive so that a and {A} are not the same variable. Any other characters are considered to be either mathematical operators or invalid, even if there is no space between the character and the rest of the variable name.

Examples of valid variable names are:

    a, dog, var1, var_2

Numbers can be integer or floating point. Scientific notation is accepted as a valid syntax. For example:

    1.0, 1.0e-2, 3.4E-4
### 10.2.2 Basic expressions

Table 10.1: Basic expressions involving unary, binary, and logical operators.

<table>
<thead>
<tr>
<th>Expression</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(exp1)</td>
<td>Parenthesis for changing precedence</td>
</tr>
<tr>
<td>+exp1</td>
<td>Unary Plus</td>
</tr>
<tr>
<td>-exp1</td>
<td>Unary Minus</td>
</tr>
<tr>
<td>!exp1</td>
<td>Logical Not</td>
</tr>
<tr>
<td>exp1 ^ exp2</td>
<td>Exponentiation</td>
</tr>
<tr>
<td>exp1 * exp2</td>
<td>Multiplication</td>
</tr>
<tr>
<td>exp1 / exp2</td>
<td>Division</td>
</tr>
<tr>
<td>exp1 + exp2</td>
<td>Addition</td>
</tr>
<tr>
<td>exp1 - exp2</td>
<td>Subtraction</td>
</tr>
<tr>
<td>exp1 &lt; exp2</td>
<td>Test Less</td>
</tr>
<tr>
<td>exp1 &lt;= exp2</td>
<td>Test Less Equal</td>
</tr>
<tr>
<td>exp1 &gt; exp2</td>
<td>Test Greater</td>
</tr>
<tr>
<td>exp1 &gt;= exp2</td>
<td>Test Greater Equal</td>
</tr>
<tr>
<td>exp1 == exp2</td>
<td>Test Equality</td>
</tr>
<tr>
<td>exp1 != exp2</td>
<td>Test Inequality</td>
</tr>
<tr>
<td>exp1 &amp;&amp; exp2</td>
<td>Logical And</td>
</tr>
<tr>
<td>exp1</td>
<td></td>
</tr>
<tr>
<td>variable</td>
<td>Independent Variable</td>
</tr>
<tr>
<td>number</td>
<td>Integer or decimal number</td>
</tr>
</tbody>
</table>

In Table 10.1, the basic syntax for the language is presented. An expression may be composed of variables and numbers tied together with mathematical operations. Order of operations is from bottom to top in order of increasing precedence. Operators with the same level of precedence are contained within horizontal lines.

In the expression `a + b * c`, the multiplication will be performed before the addition. In order to override this precedence, parenthesis may be used. For example, in `(a + b) * c`, the addition operation is performed before the multiplication.

The logical operators are based on non zero values being true and zero values being false. The test operators evaluate the numerical values and result in 0 for false and 1 for true.

*It is important to note since values are based on double precision arithmetic, testing for equality with values other than 0.0 may yield unexpected results.*
10.2.3 Functions

Table 10.2: Predefined Functions.

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>acosh(exp1)</td>
<td>Inverse Hyperbolic Cosine</td>
</tr>
<tr>
<td>asinh(exp1)</td>
<td>Inverse Hyperbolic Sine</td>
</tr>
<tr>
<td>atanh(exp1)</td>
<td>Inverse Hyperbolic Tangent</td>
</tr>
<tr>
<td>B(exp1)</td>
<td>Bernoulli Function</td>
</tr>
<tr>
<td>dBdx(exp1)</td>
<td>derivative of Bernoulli function</td>
</tr>
<tr>
<td>derfcdx(exp1)</td>
<td>derivative of complementary error function</td>
</tr>
<tr>
<td>derfdx(exp1)</td>
<td>derivative error function</td>
</tr>
<tr>
<td>dFermidx(exp1)</td>
<td>derivative of Fermi Integral</td>
</tr>
<tr>
<td>dInvFermidx(exp1)</td>
<td>derivative of InvFermi Integral</td>
</tr>
<tr>
<td>dot2d(exp1x, exp1y, exp2x, exp2y)</td>
<td>exp1x<em>exp2x+exp1y</em>exp2y</td>
</tr>
<tr>
<td>erfc(exp1)</td>
<td>complementary error function</td>
</tr>
<tr>
<td>erf(exp1)</td>
<td>error function</td>
</tr>
<tr>
<td>exp(exp1)</td>
<td>exponent</td>
</tr>
<tr>
<td>Fermi(exp1)</td>
<td>Fermi Integral</td>
</tr>
<tr>
<td>ifelse(test, exp1, exp2)</td>
<td>if test is true, then evaluate exp1, otherwise exp2</td>
</tr>
<tr>
<td>if(test, exp)</td>
<td>if test is true, then evaluate exp, otherwise 0</td>
</tr>
<tr>
<td>InvFermi(exp1)</td>
<td>inverse of the Fermi Integral</td>
</tr>
<tr>
<td>log(exp1)</td>
<td>natural log</td>
</tr>
<tr>
<td>max(exp1, exp2)</td>
<td>maximum of the two arguments</td>
</tr>
<tr>
<td>min(exp1, exp2)</td>
<td>minimum of the two arguments</td>
</tr>
<tr>
<td>pow(exp1, exp2)</td>
<td>take exp1 to the power of exp2</td>
</tr>
<tr>
<td>sgn(exp1)</td>
<td>sign function</td>
</tr>
<tr>
<td>step(exp1)</td>
<td>unit step function</td>
</tr>
<tr>
<td>kahan3(exp1, exp2, exp3)</td>
<td>Extended precision addition of arguments</td>
</tr>
<tr>
<td>kahan4(exp1, exp2, exp3, exp4)</td>
<td>Extended precision addition of arguments</td>
</tr>
<tr>
<td>vec_max</td>
<td>maximum of all the values over the entire region or interface</td>
</tr>
<tr>
<td>vec_min</td>
<td>minimum of all the values over the entire region or interface</td>
</tr>
<tr>
<td>vec_sum</td>
<td>sum of all the values over the entire region or interface</td>
</tr>
</tbody>
</table>

In Table 10.2 are the built-in functions of SYMDIFF. Note that the pow function uses the , operator to separate arguments. In addition an expression like pow(a, b+y) is equivalent to an expression like a^(b+y). Both exp and log are provided since many derivative expressions can be expressed in terms of these two functions. It is possible to nest expressions within functions and vice-versa.
10.2.4 Commands

Table 10.3: Commands.

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>diff(obj1, var)</code></td>
<td>Take derivative of <code>obj1</code> with respect to variable <code>var</code></td>
</tr>
<tr>
<td><code>expand(obj)</code></td>
<td>Expand out all multiplications into a sum of products</td>
</tr>
<tr>
<td><code>help</code></td>
<td>Print description of commands</td>
</tr>
<tr>
<td><code>scale(obj)</code></td>
<td>Get constant factor</td>
</tr>
<tr>
<td><code>sign(obj)</code></td>
<td>Get sign as 1 or -1</td>
</tr>
<tr>
<td><code>simplify(obj)</code></td>
<td>Simplify as much as possible</td>
</tr>
<tr>
<td><code>subst(obj1, obj2, obj3)</code></td>
<td>Substitute <code>obj3</code> for <code>obj2</code> into <code>obj1</code></td>
</tr>
<tr>
<td><code>unscaledval(obj)</code></td>
<td>Get value without constant scaling</td>
</tr>
<tr>
<td><code>unsignedval(obj)</code></td>
<td>Get unsigned value</td>
</tr>
</tbody>
</table>

Commands are shown in Table 10.3. While they appear to have the same form as functions, they are special in the sense that they manipulate expressions and are never present in the expression which results. For example, note the result of the following command

```plaintext
> diff(a*b, b)
a
```

10.2.5 User functions

Table 10.4: Commands for user functions.

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>clear(name)</code></td>
<td>Clears the name of a user function</td>
</tr>
<tr>
<td><code>declare(name(arg1, arg2, ...))</code></td>
<td>declare function name taking dummy arguments <code>arg1, arg2, ...</code></td>
</tr>
<tr>
<td><code>define(name(arg1, arg2, ..., obj1, obj2, ...)</code></td>
<td>declare function name taking arguments <code>arg1, arg2, ...</code> having corresponding derivatives <code>obj1, obj2, ...</code></td>
</tr>
</tbody>
</table>

Commands for specifying and manipulating user functions are listed in Table 10.4. They are used in order to define new user function, as well as the derivatives of the functions with respect to the user variables. For example, the following expression defines a function named `f` which takes one argument.

```plaintext
> define(f(x), 0.5*x)
```

The list after the function prototype is used to define the derivatives with respect to each of the independent variables. Once defined, the function may be used in any other expression. In additions the any expression can be used as an arguments. For example:

```plaintext
> diff(f(x*y), x)
(0.5 * (x * y)) * y
> simplify((0.5 * (x * y)) * y)
(0.5 * x * (y^2))
```
The chain rule is applied to ensure that the derivative is correct. This can be expressed as

\[
\frac{\partial}{\partial x} f(u, v, \ldots) = \frac{\partial u}{\partial x} \cdot \frac{\partial}{\partial u} f(u, v, \ldots) + \frac{\partial v}{\partial x} \cdot \frac{\partial}{\partial v} f(u, v, \ldots) + \ldots
\]

The `declare` command is required when the derivatives of two user functions are based on one another. For example:

```plaintext
> declare(cos(x))
cos(x)
> define(sin(x), cos(x))
sin(x)
> define(cos(x), -sin(x))
cos(x)
```

When declared, a functions derivatives are set to 0, unless specified with a `define` command. It is now possible to use these expressions as desired.

```plaintext
> diff(sin(cos(x)), x)
(cos(cos(x)) * (-sin(x)))
> simplify(cos(cos(x)) * (-sin(x)))
(-cos(cos(x)) * sin(x))
```

### 10.2.6 Macro assignment

The use of macro assignment allows the substitution of expressions into new expressions. Every time a command is successfully used, the resulting expression is assigned to a special macro definition, $\_$. In this example, the result of the each command is substituted into the next.

```plaintext
> a+b
(a + b)
> $\_ - b
((a + b) - b)
> simplify($\_)
a
```

In addition to the default macro definition, it is possible to specify a variable identifier by using the $ character followed by an alphanumeric string beginning with a letter. In addition to letters and numbers, a _ character may be used as well. A macro which has not previously assigned will implicitly use 0 as its value.

This example demonstrates the use of macro assignment.

```plaintext
> $a1 = a + b
(a + b)
> $a2 = a - b
(a - b)
> simplify($a1+$a2)
(2 * a)
```

10.2. Syntax 51
10.3 Invoking SYMDIFF from DEVSIM

10.3.1 Equation parser

The `devsim.symdiff()` (page 86) should be used when defining new functions to the parser. Since you do not specify regions or interfaces, it considers all strings as being independent variables, as opposed to models. *Model Commands* (page 76) presents commands which have the concepts of models. A `;` should be used to separate each statement.

This is a sample invocation from DEVSIM

```python
% symdiff(expr="subst(dog * cat, dog, bear)")(bear * cat)
```

10.3.2 Evaluating external math

The `devsim.register_function()` (page 85) is used to evaluate functions declared or defined within SYMDIFF. A Python procedure may then be used taking the same number of arguments. For example:

```python
from math import cos
from math import sin
symdiff(expr="declare(sin(x))")
symdiff(expr="define(cos(x), -sin(x))")
symdiff(expr="define(sin(x), cos(x))")
register_function(name="cos", nargs=1)
register_function(name="sin", nargs=1)
```

The `cos` and `sin` function may then be used for model evaluation. For improved efficiency, it is possible to create procedures written in C or C++ and load them into Python.

10.3.3 Models

When used withing the model commands discussed in *Model Commands* (page 76), DEVSIM has been extended to recognize model names in the expressions. In this situation, the derivative of a model named, `model`, with respect to another model, `variable`, is then `model:variable`.

During the element assembly process, DEVSIM evaluates all models of an equation together. While the expressions in models and their derivatives are independent, the software uses a caching scheme to ensure that redundant calculations are not performed. It is recommended, however, that users developing their own models investigate creating intermediate models in order to improve their understanding of the equations that they wish to be assembled.
Chapter 11

Visualization

11.1 Introduction

DEVSIM is able to create files for visualization tools. Information about acquiring these tools are presented in *External Software Tools* (page 57).

11.2 Using Tecplot

The `devsim.write_devices()` (page 75) is used to create an ASCII file suitable for use in Tecplot. Edge quantities are interpolated onto the node positions in the resulting structure. Element edge quantities are interpolated onto the centers of each triangle or tetrahedron in the mesh.

```
write_devices(file="mos_2d_dd.dat", type="tecplot")
```

11.3 Using Postmini

The `devsim.write_devices()` (page 75) is used to create an ASCII file suitable for use in Postmini. Edge and element edge quantities are interpolated onto the node positions in the resulting structure.

```
write_devices(file="mos_2d_dd.flps", type="floops")
```

11.4 Using Paraview

The `devsim.write_devices()` (page 75) is used to create an ASCII file suitable for use in ParaView. Edge quantities are interpolated onto the node positions in the resulting structure. Element edge quantities are interpolated onto the centers of each triangle or tetrahedron in the mesh.
write_devices(file="mos_2d_dd", type="vtk")

One vtu file per device region will be created, as well as a vtm file which may be used to load all of the device regions into ParaView.

### 11.5 Using VisIt

VisIt supports reading the Tecplot and ParaView formats. When using the vtk option on the `devsim.write_devices()` (page 75), a file with a visit filename extension is created to load the files created for ParaView.

### 11.6 DEVSIM

DEVSIM has several commands for getting information on the mesh. Those related to post processing are described in Model Commands (page 76) and Geometry Commands (page 66).

See Loading and saving results (page 40) for information about loading and saving mesh information to a file.
Chapter 12

Installation

12.1 Availability

Information about the open source version of DEVSIM is available from https://devsim.org. This site contains up-to-date information about where to obtain compiled and source code versions of this software. It also contains information about how to get support and participate in the development of this project.

12.2 Supported platforms

DEVSIM is compiled and tested on the platforms in Table 12.1. If you require a version on a different software platform, please contact us.

Table 12.1: Current platforms for DEVSIM.

<table>
<thead>
<tr>
<th>Platform</th>
<th>Bits</th>
<th>OS Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>Microsoft Windows</td>
<td>32, 64</td>
<td>Microsoft Windows 7, Microsoft Windows 10</td>
</tr>
<tr>
<td>Linux</td>
<td>64</td>
<td>Ubuntu 14.04 (LTS), Ubuntu 16.04 (LTS), Red Hat Enterprise Linux 6 (Centos 6 compatible)</td>
</tr>
<tr>
<td>Apple macOS</td>
<td>64</td>
<td>macOS 10.13 (High Sierra)</td>
</tr>
</tbody>
</table>

12.3 Binary availability

Compiled packages for the the platforms in Table 12.1 are currently available from https://github.com/devsim/devsim/releases. The prerequisites on each platform are described in the linux.txt, macos.txt, and windows.txt.
12.4 Source code availability

DEVSIM is also available in source code form from https://github.com/devsim/devsim.

12.5 Directory Structure

A DEVSIM directory is created with the following sub directories listed in Table 12.2.

<table>
<thead>
<tr>
<th>Directory</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>bin</td>
<td>contains the devsim tcl binary</td>
</tr>
<tr>
<td>lib/devsim</td>
<td>contains the devsim interpreter modules</td>
</tr>
<tr>
<td>lib/devsim/python_packages</td>
<td>contains runtime libraries</td>
</tr>
<tr>
<td>doc</td>
<td>contains product documentation</td>
</tr>
<tr>
<td>examples</td>
<td>contains example scripts</td>
</tr>
<tr>
<td>testing</td>
<td>contains additional examples used for testing</td>
</tr>
</tbody>
</table>

Table 12.2: Directory structure for DEVSIM.

12.6 Running DEVSIM

See User Interface (page 43) for instructions on how to invoke DEVSIM.
Chapter 13

Additional Information

13.1 DEVSIM License

Individual files are covered by the license terms contained in the comments at the top of the file. Contributions to this project are subject to the license terms of their authors. In general, DEVSIM is covered by the Apache License, Version 2.0 [ApacheSoftwareFoundation]. Please see the NOTICE and LICENSE file for more information.

13.2 SYMDIFF

SYMDIFF is available from https://symdiff.org under the terms of the Apache License, Version 2.0 [ApacheSoftwareFoundation].

13.3 External Software Tools

13.3.1 Genius

Genius is available in commercial and open source versions from http://www.cogenda.com.

13.3.2 Gmsh


13.3.3 Paraview

ParaView is an open source visualization tool available at http://www.paraview.org.
13.3.4 Tecplot


13.3.5 VisIt

VisIt is an open source visualization tool available from https://wci.llnl.gov/codes/visit/.

13.4 Library Availability

The following tools are used to build DEVSIM.

13.4.1 BLAS and LAPACK

These are the basic linear algebra routines used directly by DEVSIM and by SuperLU. Reference versions are available from http://www.netlib.org. There are optimized versions available from other vendors.

13.4.2 CGNS

CGNS (CFD Generalized Notation System) is an open source library, which implements the storage format used to read Genius Device Simulator meshes. It is available from http://www.cgns.org.

13.4.3 Python

A Python distribution is required for using DEVSIM and is distributed with many operating system. Additional information is available at https://www.python.org. It should be stressed that binary packages must be compatible with the Python distribution used by DEVSIM.

13.4.4 SQLite3

SQLite3 is an open source database engine used for the material database and is available from https://www.sqlite.org.

13.4.5 SuperLU

SuperLU [DEG+99] is used within DEVSIM and is available from http://crd-legacy.lbl.gov/~xiaoye/SuperLU:

Copyright (c) 2003, The Regents of the University of California, through Lawrence Berkeley National Laboratory (subject to receipt of any required approvals from U.S. Dept. of Energy)

All rights reserved.
Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

(1) Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer. (2) Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution. (3) Neither the name of Lawrence Berkeley National Laboratory, U.S. Dept. of Energy nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

13.4.6 Tcl

Tcl is the original parser for DEVSIM and is superseded by Python. It is still used for some of the tests. Tcl is available from http://www.tcl.tk.

13.4.7 zlib

zlib is an open source compression library available from https://zlib.net.
Chapter 14

Command Reference

14.1 Circuit Commands

Commands are for adding circuit elements to the simulation.

```python
devsim.add_circuit_node(**kwargs)
    Adds a circuit node for use in circuit or multi-device simulation

Parameters
    name [str] Name of the circuit node being created
    value [Float, optional] initial value (default 0.0)
    variable_update [{‘default’, ‘log_damp’, ‘positive’}] update type for circuit variable
```

```python
devsim.circuit_alter(**kwargs)
    Alter the value of a circuit element parameter

Parameters
    name [str] Name of the circuit node being created
    param [str, optional] parameter being modified (default ‘value’)
    value [Float] value for the parameter
```

```python
devsim.circuit_element(**kwargs)
    Adds a circuit element external to the devices

Parameters
    value [Float, optional] value for the default parameter of the circuit element (default 0.0)
    n1 [str] circuit node
```
n2 [str] circuit node
acreal [Float, optional] real part of AC source for voltage (default 0.0)
acimag [Float, optional] imag part of AC source for voltage (default 0.0)

devsim.circuit_node_alias(**kwargs)
    Create an alias for a circuit node
    
    Parameters
    
    node [str] circuit node being aliased
    alias [str] alias for the circuit node

devsim.get_circuit_equation_number(**kwargs)
    Returns the row number correspond to circuit node in a region. Values are only valid when during the course of a solve.
    
    Parameters
    
    node [str] circuit node

devsim.get_circuit_node_list(**kwargs)
    Gets the list of the nodes in the circuit.

devsim.get_circuit_node_value(**kwargs)
    Gets the value of a circuit node for a given solution type.
    
    Parameters
    
    solution [str, optional] name of the solution. ‘dcop’ is the name for the DC solution (default ‘dcop’)
    node [str] circuit node of interest

devsim.get_circuit_solution_list(**kwargs)
    Gets the list of available circuit solutions.

devsim.set_circuit_node_value(**kwargs)
    Sets the value of a circuit node for a given solution type.
    
    Parameters
    
    solution [str, optional] name of the solution. ‘dcop’ is the name for the DC solution (default ‘dcop’)
    node [str] circuit node of interest
    value [Float, optional] new value (default 0.0)

14.2 Equation Commands

Commands for manipulating equations on contacts, interface, and regions

devsim.contact_equation(**kwargs)
    Create a contact equation on a device
Parameters

device [str] The selected device

contact [str] Contact on which to apply this command

name [str] Name of the contact equation being created

variable_name [str, optional] The variable name is used to determine the bulk equation we are replacing at this contact (deprecated)

circuit_node [str, optional] Name of the circuit we integrate the flux into

derge_charge_model [str, optional] Name of the edge model used to determine the charge at this contact

derge_current_model [str, optional] Name of the edge model used to determine the current flowing out of this contact

derge_model [str, optional] Name of the edge model being integrated at each edge at this contact

derelement_charge_model [str, optional] Name of the element edge model used to determine the charge at this contact

derelement_current_model [str, optional] Name of the element edge model used to determine the current flowing out of this contact

derelement_model [str, optional] Name of the element edge model being integrated at each edge at this contact

dnode_charge_model [str, optional] Name of the node model used to determine the charge at this contact

dnode_current_model [str, optional] Name of the node model used to determine the current flowing out of this contact

dnode_model [str, optional] Name of the node_model being integrated at each node at this contact

devsim.custom_equation(**kwargs)

Custom equation assembly. See Custom matrix assembly (page 30) for a description of how the function should be structured.

Parameters

name [str] Name of the custom equation being created

procedure [str] The procedure to be called

devsim.delete_contact_equation(**kwargs)

This command deletes an equation from a contact.

Parameters

device [str] The selected device

contact [str] Contact on which to apply this command
**name** [str] Name of the contact equation being deleted

devsim.delete_equation(**kwargs)
This command deletes an equation from a region.

**Parameters**

**device** [str] The selected device

**region** [str] The selected region

**name** [str] Name of the equation being deleted

devsim.delete_interface_equation(**kwargs)
This command deletes an equation from an interface.

**Parameters**

**device** [str] The selected device

**interface** [str] Interface on which to apply this command

**name** [str] Name of the interface equation being deleted

devsim.equation(**kwargs)
Specify an equation to solve on a device

**Parameters**

**device** [str] The selected device

**region** [str] The selected region

**name** [str] Name of the equation being created

**variable_name** [str] Name of the node_solution being solved

**node_model** [str, optional] Name of the node_model being integrated at each node in the device volume

**edge_model** [str, optional] Name of the edge model being integrated over each edge in the device volume

**edge_volume_model** [str, optional] Name of the edge model being integrated over the volume of each edge in the device volume

**time_node_model** [str, optional] Name of the time dependent node_model being integrated at each node in the device volume

**element_model** [str, optional] Name of the element_model being integrated over each edge in the device volume

**volume_model** [str, optional] Name of the element_model being integrated over the volume of each edge in the device volume

**variable_update** [str, optional] update type for circuit variable (default ‘default’)
Notes

The integration variables can be changed in 2D for cylindrical coordinate systems by setting the appropriate parameters as described in Cylindrical Coordinate Systems (page 31).

In order to set the node volumes for integration of the `edge_volume_model`, it is possible to do something like this:

```python
devsim.get_contact_equation_command(**kwargs)
```
This command gets the options used when creating this contact equation.

**Parameters**

- `device` [str] The selected device
- `contact` [str] Contact on which to apply this command
- `name` [str] Name of the contact equation being command options returned

```python
devsim.get_contact_equation_list(**kwargs)
```
This command gets a list of equations on the specified contact.

**Parameters**

- `device` [str] The selected device
- `contact` [str] Contact on which to apply this command

```python
devsim.get_equation_command(**kwargs)
```
This command gets the options used when creating this equation.

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region
- `name` [str] Name of the equation being command options returned

```python
devsim.get_equation_list(**kwargs)
```
This command gets a list of equations on the specified region.

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region

```python
devsim.get_equation_numbers(**kwargs)
```
Returns a list of the equation numbers corresponding to each node in a region. Values are only valid when during the course of a solve.

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region
- `equation` [str, optional] Name of the equation

14.2. Equation Commands 65
variable  [str, optional] Name of the variable

devsim.get_interface_equation_command(**kwargs)
This command gets the options used when creating this interface equation.

Parameters

device  [str] The selected device

interface  [str] Interface on which to apply this command

name  [str] Name of the interface equation being command options returned

devsim.get_interface_equation_list(**kwargs)
This command gets a list of equations on the specified interface.

Parameters

device  [str] The selected device

interface  [str] Interface on which to apply this command

devsim.interface_equation(**kwargs)
Command to specify an equation at an interface

Parameters

device  [str] The selected device

interface  [str] Interface on which to apply this command

name  [str] Name of the interface equation being created

name0  [str, optional] Name of the equation coupling in region 0 being created (default ‘name’)

name1  [str, optional] Name of the equation coupling in region 1 being created (default ‘name’)

variable_name  [str, optional] The variable name is used to determine the bulk equation we are coupling this interface to (deprecated)

interface_model  [str] When specified, the bulk equations on both sides of the interface are integrated together. This model is then used to specify how nodal quantities on both sides of the interface are balanced

type  [str] Specifies the type of boundary condition

14.3 Geometry Commands

Commands for getting information about the device structure.

devsim.get_contact_list(**kwargs)
Gets a list of contacts on a device.

Parameters
device [str] The selected device

devsim.get_device_list(**kwargs)
Gets a list of devices on the simulation.

devsim.get_element_node_list(**kwargs)
Gets a list of nodes for each element on a device, region, contact, or interface.

Parameters

device [str] The selected device
region [str] The selected region
contact [str, optional] If specified, gets the element nodes for the contact on the specified region
interface [str, optional] If specified, gets the element nodes for the interface on the specified region

devsim.get_interface_list(**kwargs)
Gets a list of interfaces on a device.

Parameters

device [str] The selected device

devsim.get_region_list(**kwargs)
Gets a list of regions on a device, contact, or interface.

Parameters

device [str] The selected device
contact [str, optional] If specified, gets the name of the region belonging to this contact on the device
interface [str, optional] If specified, gets the name of the regions belonging to this interface on the device

14.4 Material Commands

Commands for manipulating parameters and material properties

devsim.add_db_entry(**kwargs)
Adds an entry to the database

Parameters

material [str] Material name requested. global refers to all regions whose material does not have the parameter name specified
parameter [str] Parameter name
value [str] Value assigned for the parameter
unit [str] String describing the units for this parameter name
description [str] Description of the parameter for this material type.

Notes

The `devsim.save_db()` (page 69) command is used to commit these added entries permanently to the database.

`devsim.close_db(**kwargs)`
Closes the database so that its entries are no longer available.

`devsim.create_db(**kwargs)`
Create a database to store material properties

Parameters

  filename [str] filename to create for the db

`devsim.get_db_entry(**kwargs)`
This command returns a list containing the value, unit, and description for the requested material db entry

Parameters

  material [str] Material name
  parameter [str] Parameter name

`devsim.get_dimension(**kwargs)`
Get the dimension of the device

Parameters

  device [str, optional] The selected device

`devsim.get_material(**kwargs)`
Returns the material for the specified region

Parameters

  device [str, optional] The selected device
  region [str, optional] The selected region
  contact [str, optional] Contact on which to apply this command

`devsim.get_parameter(**kwargs)`
Get a parameter on a region, device, or globally.

Parameters

  device [str, optional] The selected device
  region [str, optional] The selected region
  name [str] Name of the parameter name being retrieved
**Notes**

Note that the `device` and `region` options are optional. If the region is not specified, the parameter is retrieved for the entire device. If the device is not specified, the parameter is retrieved for all devices. If the parameter is not found on the region, it is retrieved on the device. If it is not found on the device, it is retrieved over all devices.

```python
devsim.get_parameter_list(**kwargs)
Get list of parameter names on region, device, or globally
```

**Parameters**

- `device` [str, optional] The selected device
- `region` [str, optional] The selected region

**Notes**

Note that the `device` and `region` options are optional. If the region is not specified, the parameter is retrieved for the entire device. If the device is not specified, the parameter is retrieved for all devices. Unlike the `devsim.getParameter()`, parameter names on the device are not retrieved if they do not exist on the region. Similarly, the parameter names over all devices are not retrieved if they do not exist on the device.

```python
devsim.open_db(**kwargs)
Open a database storing material properties
```

**Parameters**

- `filename` [str] filename to create for the db
- `permissions` [str, optional] permissions on the db (default ‘readonly’)

```python
devsim.save_db(**kwargs)
Saves any new or modified db entries to the database file
```

```python
devsim.set_material(**kwargs)
Sets the new material for a region
```

**Parameters**

- `device` [str, optional] The selected device
- `region` [str, optional] The selected region
- `contact` [str, optional] Contact on which to apply this command
- `material` [str] New material name

```python
devsim.set_parameter(**kwargs)
Set a parameter on region, device, or globally
```

**Parameters**

- `device` [str, optional] The selected device
region [str, optional] The selected region
name [str] Name of the parameter name being retrieved
value [any] value to set for the parameter

Notes

Note that the device and region options are optional. If the region is not specified, the parameter is set for the entire device. If the device is not specified, the parameter is set for all devices.

14.5 Meshing Commands

Commands for reading and writing meshes

devisim.add_1d_contact(**kwargs)
   Add a contact to a 1D mesh

   Parameters
   
   material [str] material for the contact being created
   mesh [str] Mesh to add the contact to
   name [str] Name for the contact being created
   tag [str] Text label for the position to add the contact


devisim.add_1d_interface(**kwargs)
   Add an interface to a 1D mesh

   Parameters
   
   mesh [str] Mesh to add the interface to
   tag [str] Text label for the position to add the interface
   name [str] Name for the interface being created


devisim.add_1d_mesh_line(**kwargs)
   Add a mesh line to a 1D mesh

   Parameters
   
   mesh [str] Mesh to add the line to
   tag [str, optional] Text label for the position
   pos [str] Position for the mesh point
   ns [Float, optional] Spacing from this point in the negative direction (default ps value)
   ps [Float] Spacing from this point in the positive direction


devisim.add_1d_region(**kwargs)
   Add a region to a 1D mesh
Parameters

mesh [str] Mesh to add the line to

tag1 [str] Text label for the position bounding the region being added

tag2 [str] Text label for the position bounding the region being added

region [str] Name for the region being created

material [str] Material for the region being created

devsim.add_2d_contact(**kwargs)

Add an interface to a 2D mesh

Parameters

name [str] Name for the contact being created

material [str] material for the contact being created

mesh [str] Mesh to add the contact to

region [str] Name of the region included in the contact

xl [Float, optional] x position for corner of bounding box (default -MAXDOUBLE)

xh [Float, optional] x position for corner of bounding box (default +MAXDOUBLE)

yl [Float, optional] y position for corner of bounding box (default -MAXDOUBLE)

yh [Float, optional] y position for corner of bounding box (default +MAXDOUBLE)

bloat [Float, optional] Extend bounding box by this amount when search for mesh to include in region (default 1e-10)

devsim.add_2d_interface(**kwargs)

Add an interface to a 2D mesh

Parameters

mesh [str] Mesh to add the interface to

name [str] Name for the interface being created

region0 [str] Name of the region included in the interface

region1 [str] Name of the region included in the interface

xl [Float, optional] x position for corner of bounding box (default -MAXDOUBLE)

xh [Float, optional] x position for corner of bounding box (default +MAXDOUBLE)

yl [Float, optional] y position for corner of bounding box (default -MAXDOUBLE)

yh [Float, optional] y position for corner of bounding box (default +MAXDOUBLE)

bloat [Float, optional] Extend bounding box by this amount when search for mesh to include in region (default 1e-10)

devsim.add_2d_mesh_line(**kwargs)

Add a mesh line to a 2D mesh
Parameters

mesh [str] Mesh to add the line to
pos [str] Position for the mesh point
ns [Float] Spacing from this point in the negative direction
ps [Float] Spacing from this point in the positive direction

devsim.add_2d_region(**kwargs)
Add a region to a 2D mesh

Parameters

mesh [str] Mesh to add the region to
region [str] Name for the region being created
material [str] Material for the region being created
xl [Float, optional] x position for corner of bounding box (default -MAXDOUBLE)
xh [Float, optional] x position for corner of bounding box (default +MAXDOUBLE)
yl [Float, optional] y position for corner of bounding box (default -MAXDOUBLE)
yh [Float, optional] y position for corner of bounding box (default +MAXDOUBLE)
bloat [Float, optional] Extend bounding box by this amount when search for mesh to include in region (default 1e-10)

devsim.add_genius_contact(**kwargs)
Create a contact for an imported Genius mesh

Parameters

genius_name [str] boundary condition name in the Genius CGNS file
material [str] material for the contact being created
mesh [str] name of the mesh being generated
name [str] name of the contact begin created
region [str] region that the contact is attached to

devsim.add_genius_interface(**kwargs)
Create an interface for an imported Genius mesh

Parameters

genius_name [str] boundary condition name in the Genius CGNS file
mesh [str] name of the mesh being generated
name [str] name of the interface begin created
region0 [str] first region that the interface is attached to
region1 [str] second region that the interface is attached to
devsim.add_genius_region(**kwargs)
Create a region for an imported Genius mesh

Parameters

- genius_name [str] region name in the Genius CGNS file
- mesh [str] name of the mesh being generated
- region [str] name of the region begin created
- material [str] material for the region being created

devsim.add_gmsh_contact(**kwargs)
Create a mesh to import a Gmsh mesh

Parameters

- gmsh_name [str] physical group name in the Gmsh file
- material [str] material for the contact being created
- mesh [str] name of the mesh being generated
- name [str] name of the contact begin created
- region [str] region that the contact is attached to

devsim.add_gmsh_interface(**kwargs)
Create an interface for an imported Gmsh mesh

Parameters

- gmsh_name [str] physical group name in the Gmsh file
- mesh [str] name of the mesh being generated
- name [str] name of the interface begin created
- region0 [str] first region that the interface is attached to
- region1 [str] second region that the interface is attached to

devsim.add_gmsh_region(**kwargs)
Create a region for an imported Gmsh mesh

Parameters

- gmsh_name [str] physical group name in the Gmsh file
- mesh [str] name of the mesh being generated
- region [str] name of the region begin created
- material [str] material for the region being created

devsim.create_1d_mesh(**kwargs)
Create a mesh to create a 1D device

Parameters

- mesh [str] name of the 1D mesh being created
devsim.\texttt{create\_2d\_mesh}(**\textit{kwargs})

Create a mesh to create a 2D device

\textbf{Parameters}

- \texttt{mesh} [str] name of the 2D mesh being created

devsim.\texttt{create\_contact\_from\_interface}(**\textit{kwargs})

Creates a contact on a device from an existing interface

\textbf{Parameters}

- \texttt{device} [str] The selected device
- \texttt{region} [str] The selected region
- \texttt{interface} [str] Interface on which to apply this command
- \texttt{material} [str] material for the contact being created
- \texttt{name} [str] name of the contact being created

devsim.\texttt{create\_device}(**\textit{kwargs})

Create a device from a mesh

\textbf{Parameters}

- \texttt{mesh} [str] name of the mesh being used to create a device
- \texttt{device} [str] name of the device being created

devsim.\texttt{create\_genius\_mesh}(**\textit{kwargs})

This command reads in a Genius mesh written in the CGNS format

\textbf{Parameters}

- \texttt{file} [str] name of the Genius mesh file being read into DEVSIM
  - \texttt{mesh} [str] name of the mesh being generated

**Notes**

If successful, this command will return a dictionary containing information about the regions and boundaries in the mesh. Please see the example in \textit{Genius} (page 39) for an example of how this information can be used for adding contacts and interfaces to the structure being created.

If the CGNS file was created with HDF as the underlying storage format, it may be necessary to convert it to ADF using the \texttt{hdf2adf} command before reading it into DEVSIM. This command is available as part of the CGNS library when it is compiled with HDF support. Please see \textit{CGNS} (page 58) for availability.

devsim.\texttt{create\_gmsh\_mesh}(**\textit{kwargs})

Create a mesh to import a Gmsh mesh

\textbf{Parameters}

- \texttt{mesh} [str] name of the mesh being generated
file  [str, optional] name of the Gmsh mesh file being read into DEVSIM
coordinates  [list, optional] List of coordinate positions on mesh.
elements  [list, optional] List of elements on the mesh.
physical_names  [list, optional] List of names for each contact, interface, and region on mesh.

Notes

This file will import a Gmsh format mesh from a file. Alternatively, the mesh structure may be passed in as arguments:

coordinates  is a float list of positions in the mesh. Each coordinate adds an x, y, and z position so that the coordinate list length is 3 times the number of coordinates.

physical_names  is a list of contact, interface, and region names. It is referenced by index by the elements list.

elements  is a list of elements. Each element adds
• Element Type (float)
  – 0 node
  – 1 edge
  – 2 triangle
  – 3 tetrahedron
• Physical Index
  – This indexes into the physical_names list.
• Nodes
  – Each node of the element indexes into the coordinates list.

devsim.finalize_mesh(**kwargs)
Finalize a mesh so no additional mesh specifications can be added and devices can be created.

Parameters

  mesh  [str] Mesh to finalize

devsim.load_devices(**kwargs)
Load devices from a DEVSIM file

Parameters

  file  [str] name of the file to load the meshes from

devsim.write_devices(**kwargs)
Write a device to a file for visualization or restart

Parameters
file [str] name of the file to write the meshes to
device [str, optional] name of the device to write
type [{‘devsim’, ‘devsim_data’, ‘floops’, ‘tecplot’, ‘vtk’}] format to use

14.6 Model Commands

Commands for defining and evaluating models

```python
devsim.contact_edge_model(**kwargs)
```
Create an edge model evaluated at a contact

Parameters

- device [str] The selected device
- contact [str] Contact on which to apply this command
- name [str] Name of the contact edge model being created
- equation [str] Equation used to describe the contact edge model being created
- display_type [{‘vector’, ‘nodisplay’, ‘scalar’}] Option for output display in graphical viewer

```python
devsim.contact_node_model(**kwargs)
```
Create an node model evaluated at a contact

Parameters

- device [str] The selected device
- contact [str] Contact on which to apply this command
- name [str] Name of the contact node model being created
- equation [str] Equation used to describe the contact node model being created
- display_type [{‘scalar’, ‘nodisplay’}] Option for output display in graphical viewer

```python
devsim.cylindrical_edge_coupler(**kwargs)
```
This command creates the EdgeCouple model for 2D cylindrical simulation

Parameters

- device [str] The selected device
- region [str] The selected region

Notes

This model is only available in 2D. The created variables are

- `ElementCylindricalEdgeCouple` (Element Edge Model)
- `CylindricalEdgeCouple` (Edge Model)
The `devsim.set_parameter()` (page 69) must be used to set

- `raxis_variable`, the variable (x or y) which is the radial axis variable in the cylindrical coordinate system
- `raxis_zero`, the location of the z axis for the radial axis variable

`devsim.cylindrical_node_volume(**kwargs)`

This command creates the `NodeVolume` model for 2D cylindrical simulation

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region

**Notes**

This model is only available in 2D. The created variables are

- `ElementCylindricalNodeVolume@en0` (Element Edge Model)
- `ElementCylindricalNodeVolume@en1` (Element Edge Model)
- `CylindricalEdgeNodeVolume@n0` (Edge Model)
- `CylindricalEdgeNodeVolume@n1` (Edge Model)
- `CylindricalNodeVolume` (Node Model)

The `ElementCylindricalNodeVolume@en0` and `ElementCylindricalNodeVolume@en1` represent the node volume at each end of the element edge.

The `devsim.set_parameter()` (page 69) must be used to set

- `raxis_variable`, the variable (x or y) which is the radial axis variable in the cylindrical coordinate system
- `raxis_zero`, the location of the z axis for the radial axis variable

`devsim.cylindrical_surface_area(**kwargs)`

This command creates the `SurfaceArea` model for 2D cylindrical simulation

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region

**Notes**

This model is only available in 2D. The created variables are

- `CylindricalSurfaceArea` (Node Model)
and is the cylindrical surface area along each contact and interface node in the device region.

The `devsim.set_parameter()` (page 69) must be used to set

- `raxis_variable`, the variable (x or y) which is the radial axis variable in the cylindrical coordinate system
- `raxis_zero`, the location of the z axis for the radial axis variable

`devsim.debug_triangle_models(**kwargs)`
Debugging command used in the development of DEVSIM and used in regressions.

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region

`devsim.delete_edge_model(**kwargs)`
Deletes an edge model from a region

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region
- `name` [str] Name of the edge model being deleted

`devsim.delete_element_model(**kwargs)`
Deletes a element model from a region

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region
- `name` [str] Name of the node model being deleted

`devsim.delete_interface_model(**kwargs)`
Deletes an interface model from an interface

**Parameters**

- `device` [str] The selected device
- `interface` [str] Interface on which to apply this command
- `name` [str] Name of the interface model being deleted

`devsim.delete_node_model(**kwargs)`
Deletes a node model from a region

**Parameters**

- `device` [str] The selected device
- `region` [str] The selected region
- `name` [str] Name of the node model being deleted
devsim.edge_average_model(**kwargs)

Creates an edge model based on the node model values

Parameters

device [str] The selected device
region [str] The selected region
node_model [str] The node model from which we are creating the edge model. If derivative is specified, the edge model is created from nodeModel:derivativeModel
edge_model [str] The edge model name being created. If derivative is specified, the edge models created are edgeModel:derivativeModel@n0 edgeModel:derivativeModel@n1, which are the derivatives with respect to the derivative model on each side of the edge
derivative [str, optional] The node model of the variable for which the derivative is being taken. The node model nodeModel:derivativeModel is used to create the resulting edge models.
average_type [str, optional] The node models on both sides of the edge are averaged together to create one of the following types of averages. (default ‘arithmetic’)

Notes

For a node model, creates 2 edge models referring to the node model value at both ends of the edge. For example, to calculate electric field:

```python
devsim.edge_average_model(device=device, region=region, node_model="Potential", edge_model="ElectricField", average_type="negative_gradient")
```

and the derivatives ElectricField:Potential@n0 and ElectricField:Potential@n1 are then created from

```python
devsim.edge_average_model(device=device, region=region, node_model="Potential", edge_model="ElectricField", average_type="negative_gradient", derivative="Potential")
```

devsim.edge_from_node_model(**kwargs)

For a node model, creates an 2 edge models referring to the node model value at both ends of the edge.

Parameters

device [str] The selected device
region [str] The selected region
node_model [str] The node model from which we are creating the edge model

Notes

For example, to calculate electric field:
devsim.edge_from_node_model(device=device, region=region, node_model="Potential")

**devsim.edge_model(**kwargs)

Creates an edge model based on an equation

**Parameters**

- **device** [str] The selected device
- **region** [str] The selected region
- **name** [str] Name of the edge model being created
- **equation** [str] Equation used to describe the edge model being created
- **display_type** [str, optional] Option for output display in graphical viewer (default ‘scalar’)

**Notes**

The vector option uses an averaging scheme for the edge values projected in the direction of each edge. For a given model, **model**, the generated components in the visualization files is:

- **model_x_onNode**
- **model_y_onNode**
- **model_z_onNode** (3D)

This averaging scheme does not produce accurate results, and it is recommended to use the **devsim.element_from_edge_model()** (page 80) to create components better suited for visualization. See **Visualization** (page 53) for more information about creating data files for external visualization programs.

**devsim.edge_solution(**kwargs)

Create node model whose values are set.

**Parameters**

- **device** [str] The selected device
- **region** [str] The selected region
- **name** [str] Name of the solution being created

**devsim.element_from_edge_model(**kwargs)

Creates element edge models from an edge model

**Parameters**

- **device** [str] The selected device
- **region** [str] The selected region
- **edge_model** [str] The edge model from which we are creating the element model
- **derivative** [str, optional] The variable we are taking with respect to edge_model
Notes

For an edge model `emodel`, creates an element models referring to the directional components on each edge of the element:

- `emodel_x`
- `emodel_y`

If the derivative variable option is specified, the `emodel@n0` and `emodel@n1` are used to create:

- `emodel_x:variable@en0`
- `emodel_y:variable@en0`
- `emodel_x:variable@en1`
- `emodel_y:variable@en1`
- `emodel_x:variable@en2`
- `emodel_y:variable@en2`

in 2D for each node on a triangular element. and

- `emodel_x:variable@en0`
- `emodel_y:variable@en0`
- `emodel_z:variable@en0`
- `emodel_x:variable@en1`
- `emodel_y:variable@en1`
- `emodel_z:variable@en1`
- `emodel_x:variable@en2`
- `emodel_y:variable@en2`
- `emodel_z:variable@en2`
- `emodel_x:variable@en3`
- `emodel_y:variable@en3`
- `emodel_z:variable@en3`

in 3D for each node on a tetrahedral element.

The suffix `en0` refers to the first node on the edge of the element and `en1` refers to the second node. `en2` and `en3` specifies the derivatives with respect the variable at the nodes opposite the edges on the element being considered.

`devsim.element_from_node_model(**kwargs)`

Creates element edge models from a node model

Parameters
device  [str] The selected device
region  [str] The selected region
node_model  [str] The node model from which we are creating the edge model

Notes

This command creates an element edge model from a node model so that each corner of the element is represented. A node model, nmodel, would be accessible as

- nmodel@en0
- nmodel@en1
- nmodel@en2
- nmodel@en3 (3D)

where en0, and en1 refer to the nodes on the element’s edge. In 2D, en2 refers to the node on the triangle node opposite the edge. In 3D, en2 and en3 refer to the nodes on the nodes off the element edge on the tetrahedral element.

devsim.element_model(**kwargs)
Create a model evaluated on element edges.

Parameters

device  [str] The selected device
region  [str] The selected region
name  [str] Name of the element edge model being created
equation  [str] Equation used to describe the element edge model being created
display_type  [str, optional] Option for output display in graphical viewer (default ‘scalar’)

devsim.element_solution(**kwargs)
Create node model whose values are set.

Parameters

device  [str] The selected device
region  [str] The selected region
name  [str] Name of the solution being created

devsim.get_edge_model_list(**kwargs)
Returns a list of the edge models on the device region

Parameters

device  [str] The selected device
region  [str] The selected region
devsim.get_edge_model_values(**kwargs)
Get the edge model values calculated at each edge.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the edge model values being returned as a list

devsim.get_element_model_list(**kwargs)
Returns a list of the element edge models on the device region

Parameters

device [str] The selected device
region [str] The selected region

devsim.get_element_model_values(**kwargs)
Get element model values at each element edge

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the element edge model values being returned as a list

devsim.get_interface_model_list(**kwargs)
Returns a list of the interface models on the interface

Parameters

device [str] The selected device
interface [str] Interface on which to apply this command

devsim.get_interface_model_values(**kwargs)
Gets interface model values evaluated at each interface node.

Parameters

device [str] The selected device
interface [str] Interface on which to apply this command
name [str] Name of the interface model values being returned as a list

devsim.get_node_model_list(**kwargs)
Returns a list of the node models on the device region

Parameters

device [str] The selected device
region [str] The selected region

---

14.6. Model Commands 83
devsim.get_node_model_values(**kwargs)
Get node model values evaluated at each node in a region.

Parameters

- **device** [str] The selected device
- **region** [str] The selected region
- **name** [str] Name of the node model values being returned as a list

devsim.interface_model(**kwargs)
Create an interface model from an equation.

Parameters

- **device** [str] The selected device
- **interface** [str] Interface on which to apply this command
- **equation** [str] Equation used to describe the interface node model being created

devsim.interface_normal_model(**kwargs)
Creates edge models whose components are based on direction and distance to an interface

Parameters

- **device** [str] The selected device
- **region** [str] The selected region
- **interface** [str] Interface on which to apply this command

Notes

This model creates the following edge models:

- **iname_distance**
- **iname_normal_x** (2D and 3D)
- **iname_normal_y** (2D and 3D)
- **iname_normal_z** (3D only)

where **iname** is the name of the interface. The normals are of the closest node on the interface. The sign is toward the interface.

devsim.node_model(**kwargs)
Create a node model from an equation.

Parameters

- **device** [str] The selected device
- **region** [str] The selected region
- **name** [str] Name of the node model being created
equation [str] Equation used to describe the node model being created
display_type [str, optional] Option for output display in graphical viewer (default ‘scalar’)

devsim.node_solution(**kwargs)
Create node model whose values are set.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the solution being created

devsim.print_edge_values(**kwargs)
Print edge values for debugging.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the edge model values being printed to the screen

devsim.print_element_values(**kwargs)
Print element values for debugging.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the element edge model values being printed to the screen

devsim.print_node_values(**kwargs)
Print node values for debugging.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the node model values being printed to the screen

devsim.register_function(**kwargs)
This command is used to register a new Python procedure for evaluation by SYMDIFF.

Parameters

name [str] Name of the function
nargs [str] Number of arguments to the function
procedure [str] The procedure to be called
devsim.set_edge_values(**kwargs)
Set edge model values from another edge model, or a list of values.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the edge model being initialized
init_from [str, optional] Node model we are using to initialize the edge solution
values [list, optional] List of values for each edge in the region.

devsim.set_element_values(**kwargs)
Set element model values from another element model, or a list of values.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the element model being initialized
init_from [str, optional] Node model we are using to initialize the element solution
values [list, optional] List of values for each element in the region.

devsim.set_node_value(**kwargs)
A uniform value is used if index is not specified. Note that equation based node models will lose this value if their equation is recalculated.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the node model being whose value is being set
index [int] Index of node being set
value [Float] Value of node being set

devsim.set_node_values(**kwargs)
Set node model values from another node model, or a list of values.

Parameters

device [str] The selected device
region [str] The selected region
name [str] Name of the node model being initialized
init_from [str, optional] Node model we are using to initialize the node solution
values [list, optional] List of values for each node in the region.
devsim.symdiff(**kwargs)

This command returns an expression. All strings are treated as independent variables. It is primarily used for defining new functions to the parser.

Parameters

- expr [str] Expression to send to SYMDIFF

devsim.vector_element_model(**kwargs)

Create vector components from an element edge model

Parameters

- device [str] The selected device
- region [str] The selected region
- element_model [str] The element model for which we are calculating the vector components

Notes

This command creates element edge models from an element model which represent the vector components on the element edge. An element model, `emodel`, would then have

- `emodel_x`
- `emodel_y`
- `emodel_z` (3D only)

The primary use of these components are for visualization.

devsim.vector_gradient(**kwargs)

Creates the vector gradient for noise analysis

Parameters

- device [str] The selected device
- region [str] The selected region
- node_model [str] The node model from which we are creating the edge model
- calc_type [str, optional] The node model from which we are creating the edge model (default ‘default’)

Notes

Used for noise analysis. The `avoidzero` option is important for noise analysis, since a node model value of zero is not physical for some contact and interface boundary conditions. For a given node model, `model`, a node model is created in each direction:

- `model_gradx` (1D)
- `model_grady` (2D and 3D)
• model_gradz (3D)

It is important not to use these models for simulation, since DEVSIM does not have a way of evaluating the derivatives of these models. The models can be used for integrating the impedance field, and other postprocessing. The devsim.element_from_edge_model() (page 80) command can be used to create gradients for use in a simulation.

14.7 Solver Commands

Commands for simulation

devsim.get_contact_charge(**kwargs)

Get charge at the contact

Parameters

device [str] The selected device
contact [str] Contact on which to apply this command
equation [str] Name of the contact equation from which we are retrieving the charge

devsim.get_contact_current(**kwargs)

Get current at the contact

Parameters

device [str] The selected device
contact [str] Contact on which to apply this command
equation [str] Name of the contact equation from which we are retrieving the current

devsim.solve(**kwargs)

Call the solver. A small-signal AC source is set with the circuit voltage source.

Parameters

solver_type [{‘direct’, ‘iterative’}] required] Linear solver type
absolute_error [Float, optional] Required update norm in the solve (default 0.0)
relative_error [Float, optional] Required relative update in the solve (default 0.0)
charge_error [Float, optional] Relative error between projected and solved charge during transient simulation (default 0.0)
gamma [Float, optional] Scaling factor for transient time step (default 1.0)
tdelta [Float, optional] time step (default 0.0)
maximum_iterations [int, optional] Maximum number of iterations in the DC solve (default 20)
frequency [Float, optional] Frequency for small-signal AC simulation (default 0.0)
output_node [str, optional] Output circuit node for noise simulation
info [bool, optional] Solve command return convergence information (default False)
Chapter 15

Example Overview

In the following chapters, examples are presented for the use of DEVSIM to solve some simulation problems. Examples are also located in the DEVSIM distribution and their location is mentioned in *Directory structure for DEVSIM*. (page 56).

The following example directories are contained in the distribution.

15.1 capacitance

These are 1D and 2D capacitor simulations, using the internal mesher. A description of these examples is presented in *Capacitor* (page 93).

15.2 diode

This is a collection of 1D, 2D, and 3D diode structures using the internal mesher, as well as Gmsh. These examples are discussed in *Diode* (page 103).

15.3 bioapp1

This is a biosensor application.

15.4 genius

This directory has examples importing meshes from Genius Device Simulator.
15.5 vector_potential

This is a 2D magnetic field simulation solving for the magnetic potential. The simulation script is `vector_potential/twowire.py` A simulation result for two wires conducting current is shown in Fig. 15.1.

Fig. 15.1: Simulation result for solving for the magnetic potential and field. The coloring is by the $Z$ component of the magnetic potential, and the stream traces are for components of magnetic field.

15.6 mobility

This is an advanced example using electric field dependent mobility models.
Chapter 16

Capacitor

16.1 Overview

In this chapter, we present a capacitance simulations. The purpose is to demonstrate the use of DEVSIM with a rather simple example. The first example in 1D Capacitor (page 93) is called cap1d.py and is located in the examples/capacitance directory distributed with DEVSIM. In this example, we have manually taken the derivative expressions. In other examples, we will show use of SYMDIFF to create the derivatives in an automatic fashion. The second example is in 2D Capacitor (page 97).

16.2 1D Capacitor

16.2.1 Equations

In this example, we are solving Poisson’s equation. In differential operator form, the equation to be solved over the structure is:

$$\epsilon \nabla^2 \psi = 0$$

and the contact boundary equations are

$$\psi_i - V_c = 0$$

where \( \psi_i \) is the potential at the contact node and \( V_c \) is the applied voltage.

16.2.2 Creating the mesh

The following statements create a one-dimensional mesh which is 1 m long with a 0.1 m spacing. A contact is placed at 0 and 1 and are named contact1 and contact2 respectively.
from devsim import *
device="MyDevice"
region="MyRegion"

### Create a 1D mesh
###
create_1d_mesh (mesh="mesh1")
add_1d_mesh_line (mesh="mesh1", pos=0.0, ps=0.1, tag="contact1")
add_1d_mesh_line (mesh="mesh1", pos=1.0, ps=0.1, tag="contact2")
add_1d_contact (mesh="mesh1", name="contact1", tag="contact1",
    material="metal")
add_1d_contact (mesh="mesh1", name="contact2", tag="contact2",
    material="metal")
add_1d_region (mesh="mesh1", material="Si", region=region,
    tag1="contact1", tag2="contact2")
finalize_mesh (mesh="mesh1")
create_device (mesh="mesh1", device=device)

16.3 Setting device parameters

In this section, we set the value of the permittivity to that of SiO$_2$.

### Set parameters on the region
###
set_parameter(device=device, region=region,
    name="Permittivity", value=3.9*8.85e-14)

16.3.1 Creating the models

Solving for the Potential, $\psi$, we first create the solution variable.

### Create the Potential solution variable
###
node_solution(device=device, region=region, name="Potential")

In order to create the edge models, we need to be able to refer to Potential on the nodes on each edge.

### Creates the Potential@n0 and Potential@n1 edge model
###
edge_from_node_model(device=device, region=region, node_model="Potential")

We then create the ElectricField model with knowledge of Potential on each node, as well as the EdgeInverseLength of each edge. We also manually calculate the derivative of ElectricField with Potential on each node and name them ElectricField:Potential@n0 and ElectricField:Potential@n1.
### Electric field on each edge, as well as its derivatives with respect to the potential at each node

```python
def edge_model(device=device, region=region, name="ElectricField",
               equation="(Potential@n0 - Potential@n1)*EdgeInverseLength")
```

```python
def edge_model(device=device, region=region, name="ElectricField:Potential@n0",
               equation="EdgeInverseLength")
```

```python
def edge_model(device=device, region=region, name="ElectricField:Potential@n1",
               equation="-EdgeInverseLength")
```

We create `DField` to account for the electric displacement field.

```python
def edge_model(device=device, region=region, name="DField",
               equation="Permittivity*ElectricField")
```

```python
def edge_model(device=device, region=region, name="DField:Potential@n0",
               equation="diff(Permittivity*ElectricField, Potential@n0)")
```

```python
def edge_model(device=device, region=region, name="DField:Potential@n1",
               equation="-DField:Potential@n0")
```

The bulk equation is now created for the structure using the models and parameters we have previously defined.

```python
def equation(device=device, region=region, name="PotentialEquation",
            variable_name="Potential", edge_model="DField",
            variable_update="default")
```

### 16.3.2 Contact boundary conditions

We then create the contact models and equations. We use the Python for loop construct and variable substitutions to create a unique model for each contact, `contact1_bc` and `contact2_bc`.

```python
for c in ("contact1", "contact2"):  
    contact_node_model(device=device, contact=c, name="%s_bc" % c,
                        equation="Potential - %s_bias" % c)
    contact_node_model(device=device, contact=c, name="%s_bc:Potential" % c,
                        equation="")
```

(continues on next page)
In this example, the contact bias is applied through parameters named contact1_bias and contact2_bias. When applying the boundary conditions through circuit nodes, models with respect to their names and their derivatives would be required.

### 16.3.3 Setting the boundary conditions

```python
### Set the contact
set_parameter(device=device, region=region, name="contact1_bias", value=1.0e-0)
set_parameter(device=device, region=region, name="contact2_bias", value=0.0)

### Solve
solve(type="dc", absolute_error=1.0, relative_error=1e-10, maximum_iterations=30)

### Print the charge on the contacts
for c in ("contact1", "contact2"):
    print("contact: \$s charge: \$1.5e" % (c, get_contact_charge(device=device, contact=c, equation="PotentialEquation")))
```

### 16.3.4 Running the simulation

We run the simulation and see the results.

```bash
capacitance> python cap1d.py
---
DEVSIM
Version: Beta 0.01
Copyright 2009-2013 Devsim LLC
---
```
Which corresponds to our expected result of $3.451510^{-13}$ F/cm\(^2\) for a homogenous capacitor.

### 16.4 2D Capacitor

This example is called `cap2d.py` and is located in the `examples/capacitance` directory distributed with DEVSIM. This file uses the same physics as the 1D example, but with a 2D structure. The mesh is built using the DEVSIM internal mesher. An air region exists with two electrodes in the simulation domain.

### 16.5 Defining the mesh

```python
from devsim import *

device = "MyDevice"
region = "MyRegion"

xmin = -25
x1 = -24.975
x2 = -2
x3 = 2
x4 = 24.975
xmax = 25.0

ymin = 0.0
y1 = 0.1
y2 = 0.2
y3 = 0.8

(continues on next page)
y4 = 0.9
ymax = 50.0

create_2d_mesh(mesh=device)
add_2d_mesh_line(mesh=device, dir="y", pos=ymin, ps=0.1)
add_2d_mesh_line(mesh=device, dir="y", pos=y1, ps=0.1)
add_2d_mesh_line(mesh=device, dir="y", pos=y2, ps=0.1)
add_2d_mesh_line(mesh=device, dir="y", pos=y3, ps=0.1)
add_2d_mesh_line(mesh=device, dir="y", pos=y4, ps=0.1)
add_2d_mesh_line(mesh=device, dir="y", pos=ymax, ps=5.0)

device = device
region = "air"

add_2d_mesh_line(mesh=device, dir="x", pos=xmin, ps=5)
add_2d_mesh_line(mesh=device, dir="x", pos=x1, ps=2)
add_2d_mesh_line(mesh=device, dir="x", pos=x2, ps=0.05)
add_2d_mesh_line(mesh=device, dir="x", pos=x3, ps=0.05)
add_2d_mesh_line(mesh=device, dir="x", pos=x4, ps=2)
add_2d_mesh_line(mesh=device, dir="x", pos=xmax, ps=5)

add_2d_region(mesh=device, material="gas", region="air", yl=ymin, yh=ymax,
xl=xmin, xh=xmax)
add_2d_region(mesh=device, material="metal", region="m1", yl=y1, yh=y2,
xl=x1, xh=x4)
add_2d_region(mesh=device, material="metal", region="m2", yl=y3, yh=y4,
xl=x2, xh=x3)

# must be air since contacts don't have any equations
add_2d_contact(mesh=device, name="bot", region="air", material="metal", yl=y1, yh=y2, x1=x1, xh=x4)
add_2d_contact(mesh=device, name="top", region="air", material="metal", yl=y3, yh=y4, x1=x2, xh=x3)
finalize_mesh(mesh=device)
create_device(mesh=device, device=device)

16.6 Setting up the models

### Set parameters on the region
###
set_parameter(device=device, region=region, name="Permittivity", value=3.9*8.85e-14)

### Create the Potential solution variable
###
node_solution(device=device, region=region, name="Potential")
### Creates the Potential@n0 and Potential@n1 edge model

```python
edge_from_node_model(device=device, region=region, node_model="Potential")
```

### Electric field on each edge, as well as its derivatives with respect to the potential at each node

```python
def edge_model(device=device, region=region, name="ElectricField", equation="(Potential@n0 - Potential@n1)*EdgeInverseLength")

def edge_model(device=device, region=region, name="ElectricField:Potential@n0", equation="EdgeInverseLength")

def edge_model(device=device, region=region, name="ElectricField:Potential@n1", equation="-EdgeInverseLength")
```

### Model the D Field

```python
def edge_model(device=device, region=region, name="DField", equation="Permittivity*ElectricField")

def edge_model(device=device, region=region, name="DField:Potential@n0", equation="diff(Permittivity*ElectricField, Potential@n0)")

def edge_model(device=device, region=region, name="DField:Potential@n1", equation="-DField:Potential@n0")
```

### Create the bulk equation

```python
def equation(device=device, region=region, name="PotentialEquation", variable_name="Potential", edge_model="DField", variable_update="default")
```

### Contact models and equations

```python
for c in ("top", "bot"):
    contact_node_model(device=device, contact=c, name="%s_bc" % c, equation="Potential - %s_bias" % c)

    contact_node_model(device=device, contact=c, name="%s_bc:Potential" % c, equation="1")

    contact_equation(device=device, contact=c, name="PotentialEquation", variable_name="Potential", node_model="%s_bc" % c, edge_charge_model="DField")
```

(continues on next page)
### Set the contact

```python
set_parameter(device=device, name="top_bias", value=1.0e-0)
set_parameter(device=device, name="bot_bias", value=0.0)

edge_model(device=device, region="m1", name="ElectricField", equation="0")
edge_model(device=device, region="m2", name="ElectricField", equation="0")
node_model(device=device, region="m1", name="Potential", equation="bot_bias;")
node_model(device=device, region="m2", name="Potential", equation="top_bias;")

solve(type="dc", absolute_error=1.0, relative_error=1e-10, maximum_iterations=30,
solver_type="direct")
```

16.7 Fields for visualization

Before writing the mesh out for visualization, the element_from_edge_model is used to calculate the electric field at each triangle center in the mesh. The components are the ElectricField_x and ElectricField_y.

```python
element_from_edge_model(edge_model="ElectricField", device=device, region=region)
print(get_contact_charge(device=device, contact="top", equation="PotentialEquation"))
print(get_contact_charge(device=device, contact="bot", equation="PotentialEquation"))
write_devices(file="cap2d.msh", type="devsim")
write_devices(file="cap2d.dat", type="tecplot")
```

16.8 Running the simulation

```
----------------------------------------
DEVSIM
Version: Beta 0.01
Copyright 2009-2013 Devsim LLC
----------------------------------------
```
Creating Region air
Creating Region m1
Creating Region m2
Adding 8281 nodes
Adding 23918 edges with 22990 duplicates removed
Adding 15636 triangles with 0 duplicate removed
Adding 334 nodes
Adding 665 edges with 331 duplicates removed
Adding 332 triangles with 0 duplicate removed
Adding 162 nodes
Adding 321 edges with 159 duplicates removed
Adding 160 triangles with 0 duplicate removed
Contact bot in region air with 334 nodes
Contact top in region air with 162 nodes
Region "air" on device "MyDevice" has equations 0:8280
Region "m1" on device "MyDevice" has no equations.
Region "m2" on device "MyDevice" has no equations.
Device "MyDevice" has equations 0:8280
number of equations 8281
Iteration: 0
Device: "MyDevice" RelError: 1.00000e+00 AbsError: 1.00000e+00
Region: "air" RelError: 1.00000e+00 AbsError: 1.00000e+00
Equation: "PotentialEquation" RelError: 1.00000e+00 AbsError: 1.
Iteration: 1
Device: "MyDevice" RelError: 1.25144e-12 AbsError: 1.73395e-13
Region: "air" RelError: 1.25144e-12 AbsError: 1.73395e-13
3.35017166004e-12
-3.35017166004e-12
A visualization of the results is shown in Fig. 16.1.
Fig. 16.1: Capacitance simulation result. The coloring is by `Potential`, and the stream traces are for components of `ElectricField`. 
Chapter 17

Diode

The diode examples are located in the examples/diode. They demonstrate the use of packages located in the python_packages directory to simulate drift-diffusion using the Scharfetter-Gummel method [SG69].

17.1 1D diode

17.1.1 Using the python packages

For these examples, python modules are provided to supply the appropriate model and parameter settings. A listing is shown in Table 17.1. The devsim.python_packages module is part of the distribution. The example files in the DEVSIM distribution set the path properly when loading modules.

<table>
<thead>
<tr>
<th>model_create</th>
<th>Creation of models and their derivatives</th>
</tr>
</thead>
<tbody>
<tr>
<td>ramp</td>
<td>Ramping bias and automatic stepping</td>
</tr>
<tr>
<td>simple_dd</td>
<td>Functions for calculating bulk electron and hole current</td>
</tr>
<tr>
<td>simple_physics</td>
<td>Functions for setting up device physics</td>
</tr>
</tbody>
</table>

Table 17.1: Python package files.

For this example, diode_1d.py, the following line is used to import the relevant physics.

```python
from devsim import *
from simple_physics import *
```

17.1.2 Creating the mesh

This creates a mesh $10^{-6}$ cm long with a junction located at the midpoint. The name of the device is MyDevice with a single region names MyRegion. The contacts on either end are called top and bot.
def createMesh(device, region):
    create_1d_mesh(mesh="dio")
    add_1d_mesh_line(mesh="dio", pos=0, ps=1e-7, tag="top")
    add_1d_mesh_line(mesh="dio", pos=0.5e-5, ps=1e-9, tag="mid")
    add_1d_mesh_line(mesh="dio", pos=1e-5, ps=1e-7, tag="bot")
    add_1d_contact (mesh="dio", name="top", tag="top", material="metal")
    add_1d_contact (mesh="dio", name="bot", tag="bot", material="metal")
    add_1d_region (mesh="dio", material="Si", region=region, tag1="top", tag2="bot")
    finalize_mesh(mesh="dio")
    create_device(mesh="dio", device=device)

device="MyDevice"
region="MyRegion"

createMesh(device, region)

17.2 Physical Models and Parameters

#### Set parameters for 300 K
####
SetSiliconParameters(device, region, 300)
set_parameter(device=device, region=region, name="taun", value=1e-8)
set_parameter(device=device, region=region, name="taup", value=1e-8)

#### NetDoping
####
CreateNodeModel(device, region, "Acceptors", "1.0e18*step(0.5e-5-x)")
CreateNodeModel(device, region, "Donors", "1.0e18*step(x-0.5e-5)"")
CreateNodeModel(device, region, "NetDoping", "Donors-Acceptors")
print_node_values(device=device, region=region, name="NetDoping")

#### Create Potential, Potential@n0, Potential@n1
####
CreateSolution(device, region, "Potential")

#### Create potential only physical models
####
CreateSiliconPotentialOnly(device, region)

#### Set up the contacts applying a bias
####
for i in get_contact_list(device=device):
    set_parameter(device=device, name=GetContactBiasName(i), value=0.0)
    CreateSiliconPotentialOnlyContact(device, region, i)
#### Initial DC solution

```plaintext
solve(type="dc", absolute_error=1.0, relative_error=1e-12, maximum_iterations=30)
```

#### drift diffusion solution variables

```plaintext
CreateSolution(device, region, "Electrons")
CreateSolution(device, region, "Holes")
```

#### create initial guess from dc only solution

```plaintext
set_node_values(device=device, region=region, name="Electrons", init_from="IntrinsicElectrons")
set_node_values(device=device, region=region, name="Holes", init_from="IntrinsicHoles")
```

#### Set up equations

```plaintext
CreateSiliconDriftDiffusion(device, region)
for i in get_contact_list(device=device):
    CreateSiliconDriftDiffusionAtContact(device, region, i)
```

#### Drift diffusion simulation at equilibrium

```plaintext
solve(type="dc", absolute_error=1e10, relative_error=1e-10, maximum_iterations=30)
```

#### Ramp the bias to 0.5 Volts

```plaintext
v = 0.0
while v < 0.51:
    set_parameter(device=device, name=GetContactBiasName("top"), value=v)
    solve(type="dc", absolute_error=1e10, relative_error=1e-10, maximum_iterations=30)
    PrintCurrents(device, "top")
    PrintCurrents(device, "bot")
    v += 0.1
```

#### Write out the result

```plaintext
write_devices(file="diode_1d.dat", type="tecplot")
```
17.2.1 Plotting the result

A plot showing the doping profile and carrier densities are shown in Fig. 17.1. The potential and electric field distribution is shown in Fig. 17.2. The current distributions are shown in Fig. 17.3.

Fig. 17.1: Carrier density versus position in 1D diode.
Fig. 17.2: Potential and electric field versus position in 1D diode.
Fig. 17.3: Electron and hole current and recombination.
Bibliography


## Index

**A**
- add_1d_contact() *(in module devsim)*, 70
- add_1d_interface() *(in module devsim)*, 70
- add_1d_mesh_line() *(in module devsim)*, 70
- add_1d_region() *(in module devsim)*, 70
- add_2d_contact() *(in module devsim)*, 71
- add_2d_interface() *(in module devsim)*, 71
- add_2d_mesh_line() *(in module devsim)*, 71
- add_2d_region() *(in module devsim)*, 71
- add_circuit_node() *(in module devsim)*, 61
- add_db_entry() *(in module devsim)*, 67
- add_genius_contact() *(in module devsim)*, 72
- add_genius_interface() *(in module devsim)*, 72
- add_genius_region() *(in module devsim)*, 72
- add_gmsh_contact() *(in module devsim)*, 73
- add_gmsh_interface() *(in module devsim)*, 73
- add_gmsh_region() *(in module devsim)*, 73

**C**
- circuit_alter() *(in module devsim)*, 61
- circuit_element() *(in module devsim)*, 61
- circuit_node_alias() *(in module devsim)*, 62
- close_db() *(in module devsim)*, 68
- contact_edge_model() *(in module devsim)*, 76
- contact_equation() *(in module devsim)*, 62
- contact_node_model() *(in module devsim)*, 76
- create_1d_mesh() *(in module devsim)*, 73
- create_2d_mesh() *(in module devsim)*, 73
- create_contact_from_interface() *(in module devsim)*, 74
- create_db() *(in module devsim)*, 68
- create_device() *(in module devsim)*, 74
- create_genius_mesh() *(in module devsim)*, 74
- create_gmsh_mesh() *(in module devsim)*, 74
- custom_equation() *(in module devsim)*, 63
- cylindrical_edge_coupler() *(in module devsim)*, 76
- cylindrical_node_volume() *(in module devsim)*, 77
- cylindrical_surface_area() *(in module devsim)*, 77

**D**
- debug_triangle_models() *(in module devsim)*, 78
- delete_contact_equation() *(in module devsim)*, 63
- delete_edge_model() *(in module devsim)*, 78
- delete_element_model() *(in module devsim)*, 78
- delete_equation() *(in module devsim)*, 64
- delete_interface_equation() *(in module devsim)*, 64
- delete_interface_model() *(in module devsim)*, 78
- delete_node_model() *(in module devsim)*, 78
- devsim() *(module)*, 61, 62, 66, 67, 70, 76, 88

**E**
- edge_average_model() *(in module devsim)*, 78
- edge_from_node_model() *(in module devsim)*, 79
- edge_model() *(in module devsim)*, 80
- edge_solution() *(in module devsim)*, 80
- element_from_edge_model() *(in module devsim)*, 81
- element_from_node_model() *(in module devsim)*, 81
- element_model() *(in module devsim)*, 82
- element_solution() *(in module devsim)*, 82
- equation() *(in module devsim)*, 64
finalize_mesh() (in module devsim), 75

get_circuit_equation_number() (in module devsim), 62
get_circuit_node_list() (in module devsim), 62
get_circuit_node_value() (in module devsim), 62
get_circuit_solution_list() (in module devsim), 62
get_contact_charge() (in module devsim), 88
get_contact_current() (in module devsim), 88
get_contact_equation_command() (in module devsim), 65
get_contact_equation_list() (in module devsim), 65
get_contact_list() (in module devsim), 66
get_db_entry() (in module devsim), 68
get_device_list() (in module devsim), 67
get_dimension() (in module devsim), 68
get_edge_model_list() (in module devsim), 82
get_edge_model_values() (in module devsim), 82
get_element_model_list() (in module devsim), 83
get_element_model_values() (in module devsim), 83
get_element_node_list() (in module devsim), 67
get_equation_command() (in module devsim), 65
get_equation_list() (in module devsim), 65
get_equation_numbers() (in module devsim), 65
get_interface_equation_command() (in module devsim), 66
get_interface_equation_list() (in module devsim), 66
get_interface_list() (in module devsim), 67
get_interface_model_list() (in module devsim), 83
get_interface_model_values() (in module devsim), 83
get_material() (in module devsim), 68
get_node_model_list() (in module devsim), 83
get_node_model_values() (in module devsim), 83
get_parameter() (in module devsim), 68
get_parameter_list() (in module devsim), 69
get_region_list() (in module devsim), 67
interface_equation() (in module devsim), 66
interface_model() (in module devsim), 84
interface_normal_model() (in module devsim), 84
load_devices() (in module devsim), 75
node_model() (in module devsim), 84
node_solution() (in module devsim), 85
open_db() (in module devsim), 69
print_edge_values() (in module devsim), 85
print_element_values() (in module devsim), 85
print_node_values() (in module devsim), 85
register_function() (in module devsim), 85
save_db() (in module devsim), 69
set_circuit_node_value() (in module devsim), 69
set_edge_values() (in module devsim), 85
set_element_values() (in module devsim), 86
set_material() (in module devsim), 69
set_node_value() (in module devsim), 86
set_node_values() (in module devsim), 86
set_parameter() (in module devsim), 69
solve() (in module devsim), 88
symdiff() (in module devsim), 86

V
vector_element_model() (in module devsim), 87
vector_gradient() (in module devsim), 87

W
write_devices() (in module devsim), 75