DEVSIM

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Part I User Guide

Chapter 1

Release Notes

Please see *Chapter 11*, Installation *on page 67* for information on installing DEVSIM on your system. If you require assistance with this product, please contact us using the information in the front cover of this manual.

DEVSIM is now an open source distribution. The documentation is in the process of being updated to reflect this.

Chapter 2

Introduction

2.1 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.

2.2 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 is embedded within a scripting language interface (*Chapter 8*, User Interface on page 53). This provides control structures and language syntax in a consistent and intuitive manner. Taking a hierarchical approach, 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 (*Chapter 9*, SYMDIFF *on page 57*) 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.

2.3 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 Interfaces connect two regions together. At the interfaces, equations are specified to account for how the flux in each device region crosses the region boundary.

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

2.4 Equation assembly

Equation assembly of models is discussed in Chapter 3, Equation and Models on page 9.

2.5 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 *Chapter 4*, Model Parameters on page 33.

2.6 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 *Chapter 5*, Circuits on page 37.

2.7 Meshing

Meshing is discussed in Chapter 6, Meshing on page 41.

2.8 Analysis

DEVSIM offers a range of simulation algorithms. They are discussed in more detail in *Chapter 7*, Solver on page 49.

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.

2.9 Scripting interface

The scripting interface to DEVSIM is discussed in Chapter 8, User Interface on page 53.

2.10 Expression parser

The expression parser is discussed in Chapter 9, SYMDIFF on page 57.

2.11 Visualization and postprocessing

Visualization is discussed in Chapter 10, Visualization on page 65.

2.12 Installation

Installation is discussed in Chapter 11, Installation on page 67.

2.13 Additional information

Additional information is discussed in Chapter 12, Additional Information on page 69.

2.14 Examples

Examples are discused in the remaining chapters beginning with *Chapter 13*, Example Overview on page 73.

Chapter 3

Equation and Models

3.1 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:

$$\frac{\partial X}{\partial t} + \nabla \cdot \vec{Y} + Z = 0 \tag{3.1}$$

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

$$\int \frac{\partial X}{\partial t} \partial r + \int \vec{Y} \cdot \partial \vec{s} + \int Z \partial r = 0$$
(3.2)

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

In Figure 3.1, 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 *Chapter 9, SYMDIFF on page 57.* For special situations, custom matrix assembly is also available and is discussed in *Section 3.5, Custom matrix assembly on page 17.*

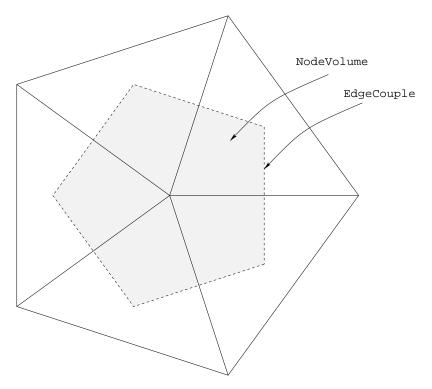


Figure 3.1: Mesh elements in 2D.

3.2 Bulk models

3.2.1 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 3.1. In this example, we present an implementation of Shockley Read Hall recombination [1].

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

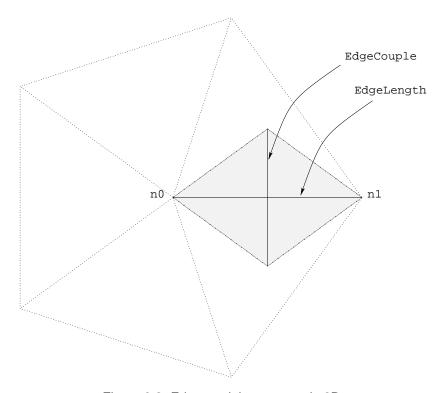


Figure 3.2: Edge model constructs in 2D.

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.

3.2.2 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 Figure 3.2, 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:

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 edge_from_node_model command (page 24). In addition, the edge_average_model command (page 24) can be used to create edge models in terms of node model quantities.

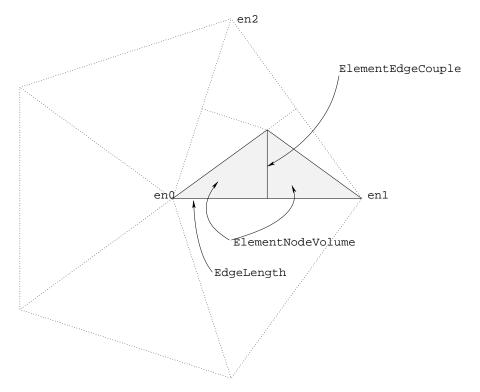


Figure 3.3: Element edge model constructs in 2D.

Edge models automatically created for a region are listed in Table 3.2.

3.2.3 Element edge models

Element edge models are used when the edge quantitites 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 Figure 3.3, 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 3.3.

As an alternative to treating integrating the element edge model with respect to ElementEdgeCouple, the integration may be performed with respect to ElementNodeVolume. See equation command (page 20) for more information.

3.2.4 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 3.4.

Node Model	Description
AtContactNode	Evaluates to 1 if node is a contact node, otherwise 0
NodeVolume	The volume of the node. Used for volume integration of node models on nodes in mesh
$NSurfaceNormal_x$	The surface normal to points on the interface or contact (2D and 3D)
NSurfaceNormal_y	The surface normal to points on the interface or contact (2D and 3D)
NSurfaceNormal_z	The surface normal to points on the interface or contact (3D)
SurfaceArea	The surface area of a node on interface and contact nodes, otherwise 0
X	x position of the node
У	y position of the node (2D and 3D)
Z	z position of the node (3D only)

Table 3.1: Node models defined on each region of a device.

Edge Model	Description		
EdgeCouple The length of the perpendicular bisector of an element edge. Used to per			
	surface integration of edge models on edges in mesh.		
EdgeInverseLength	Inverse of the EdgeLength.		
EdgeLength The distance between the two nodes of an edge			
unitx	x component of the unit vector along an edge		
unity	y component of the unit vector along an edge (2D and 3D)		
unitz	z component of the unit vector along an edge (3D only)		

Table 3.2: Edge models defined on each region of a device.

3.2.5 Conversions between model types

The edge_from_node_model command (page 24) 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 edge_average_model command (page 24) 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 implicity 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 element_from_edge_model command (page 26) 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 element_from_node_model command (page 27) is used to create element edge models referring to each node on the element of the element edge.

Element Edge Model	Description
ElementEdgeCouple	The length of the perpendicular bisector of an edge. Used to perform surface
	integration of element edge model on element edge in the mesh.
ElementNodeVolume	The node volume at either end of each element edge.

Table 3.3: Element edge models defined on each region of a device.

Model Type	Derivatives Required	
Node Model	model:variable	
Edge Model	model:variable@n0	
	model:variable@n1	
Element Edge Model	model:variable@en0	
	model:variable@en1	
	model:variable@en2	
	model:variable@en3(3D)	

Table 3.4: 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.

3.2.6 Equation assembly

Bulk equations are specified in terms of the node, edge, and element edge models using the equation command (page 20). 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.

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

3.3 Interface

3.3.1 Interface models

Figure 3.4 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 interface_model command (page 29). Interface models may

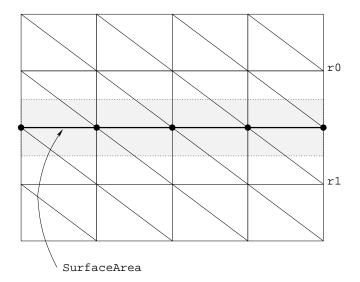


Figure 3.4: Interface constructs in 2D. Interface node pairs are located at each •. The SurfaceArea model is used to integrate flux term models.

Model Type	Model Name	Derivatives Required
Node Model (region 0)	nodemodel@r0	nodemodel:variable@r0
Node Model (region 1)	nodemodel@r1	nodemodel:variable@r1
Interface Node Model	inodemodel	inodemodel:variable@r0
		inodemodel:variable@r1

Table 3.5: 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.

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 3.5.

3.3.2 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

ds.interface_model(device="device", interface="interface",

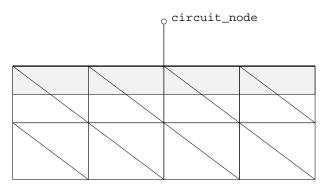


Figure 3.5: Contact constructs in 2D.

3.3.3 Interface equation assembly

There are two types of interface equations considered in DEVSIM. They are both activated using the interface_equation command (page 21).

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.

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.

3.4 Contact

3.4.1 Contact models

Figure 3.5 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 contact_node_model command (page 21) and the contact_edge_model command (page 21), respectively. The key difference is that the models are only evaluated on the contact nodes for the contact specified.

3.4.2 Contact model derivatives

The derivatives are equivalent to the discussion in Section 3.2.4, Model derivatives on page 12. If external circuit boundary conditions are being used, the model model derivative with respect to the circuit node name should be specified as model:node.

3.4.3 Contact equation assembly

The contact_equation command (page 19) 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

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

$$I(t) = i(t) + \frac{\partial q(t)}{\partial t}$$
(3.3)

where i is the integrated current and q is the integrated charge.

3.5 Custom matrix assembly

The custom_equation command (page 19) 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

```
ds.custom_equation(name="test1", procedure="myassemble")
must expect to receive two arguments
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

```
[1 1 1.0 2 2 1.0 1 2 -1.0 2 1 -1.0 2 2 1.0] [1 1.0 2 1.0 2 -1.0]
```

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 get_circuit_equation_number command (page 38) may be used to get the equation numbers corresponding to circuit node names. The get_equation_numbers command (page 20) 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.

3.6 Cylindrical Coordinate Systems

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

- cylindrical_edge_couple command (page 22)
- cylindrical_node_volume command (page 22)
- cylindrical_surface_area command (page 23)

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

```
set_parameter(name="node_volume_model", value="CylindricalNodeVolume")
set_parameter(name="edge_couple_model", value="CylindricalEdgeCouple")
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")
```

3.7 Equation commands

contact_equation

ds.contact_equation(device=STRING, contact=STRING, name=STRING,

variable_name=STRING, circuit_node=STRING,

edge_charge_model=STRING,
edge_current_model=STRING,

edge_model=STRING,

element_charge_model=STRING,
element_current_model=STRING

element_model=STRING,
node_charge_model=STRING,
node_current_model=STRING,

node_model=STRING)

device= Device on which to apply this command
contact= Contact on which to apply this command
name= Name of the contact equation being created

variable_name= The variable name is used to determine the bulk equation we are

replacing at this contact

circuit_node= Name of the circuit we integrate the flux into

edge_charge_model= Name of the edge model used to determine the charge at this contact
edge_current_model= Name of the edge model used to determine the current flowing out

of this contact

edge_model= Name of the edge model being integrated at each edge at this con-

tact

element_charge_model= Name of the element edge model used to determine the charge at

this contact

element_current_model= Name of the element edge model used to determine the current flow-

ing out of this contact

element_model= Name of the element edge model being integrated at each edge at

this contact

node_charge_model= Name of the node model used to determine the charge at this contact node_current_model= Name of the node model used to determine the current flowing out

of this contact

node_model Name of the node_model being integrated at each node at this con-

tact

custom_equation

ds.custom_equation(name=STRING, procedure=STRING)

name= Name of the custom equation being created

procedure The Python procedure to be called. See Section 3.5, Custom matrix

assembly on page 17 for a description of how the function should be

structured.

equation

device= Device on which to apply this command region= Region on which to apply this command name= Name of the equation being created variable_name= Name of the node_solution being solved

node_model = Name of the node_model being integrated at each node in the device

volume

edge_model= Name of the edge model being integrated over each edge in the

device volume

time_node_model= Name of the time dependent node_model being integrated at each

node in the device volume

element_model = Name of the element_model being integrated over each edge in the

device volume

volume_model= Name of the element_model being integrated over the volume of each

edge in the device volume

"log_damp" Variable update is damped

"positive" Solution update results in positive quantity

get_equation_numbers

device= Device on which to apply this command region= Region on which to apply this command

equation= Name of the equation (optional)
variable= Name of the variable (optional)

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.

interface_equation

ds.interface_equation(device=STRING, interface=STRING, name=STRING,

variable_name=STRING,
interface_model=STRING,

type=OPTION)

device= Device on which to apply this command
interface= Interface on which apply this command
name= Name of the interface equation being created

variable_name = The variable name is used to determine the bulk equation we are

coupling this interface to

interface_node_model= 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= Specifies the type of boundary condition

"continuous" Equations of the same name in the two regions are added. The

interface_model is an additional equation is created to specify how

quantities across the interface are solved

"fluxterm" The interface_model is added to the bulk equation in the first region,

and subtracted from the second

3.8 Model commands

contact_edge_model

device= Device on which to apply this command
contact= Contact on which to apply this command
name= Name of the contact edge model being created

equation= Equation used to describe the contact edge model being created

display_type= Option for output display in graphical viewer

"nodisplay" Data on edge will not be displayed "scalar" Data on edge is a scalar quantity

"vector" Data on edge is a vector quantity (default)

contact_node_model

device= Device on which to apply this command

contact= Contact on which to apply this command

name= Name of the contact node model being created

equation= Equation used to describe the contact node model being created

display_type= Option for output display in graphical viewer

"nodisplay" Data on node will not be displayed

"scalar" Data on node is a scalar quantity (default)

cylindrical_edge_couple

ds.cylindrical_edge_couple(device=STRING, region=STRING)

device= Device on which to apply this command
region= Region on which to apply this command

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

- ElementCylindricalEdgeCouple (Element Edge Model)
- CylindricalEdgeCouple (Edge Model)

The set_parameter command (page 34) 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

cylindrical_node_volume

device= Device on which to apply this command
region= Region on which to apply this command

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

- ElementCylindricalNodeVolume@enO (Element Edge Model)
- ElementCylindricalNodeVolume@en1 (Element Edge Model)
- CylindricalNodeVolume (Edge Model)

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

The set_parameter command (page 34) must be used to set

- ullet 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

cylindrical_surface_area

```
ds.cylindrical_surface_area(device=STRING, region=STRING)
```

device= Device on which to apply this command region= Region on which to apply this command

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 set_parameter command (page 34) 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

delete_edge_model

device= Device on which to apply this command region= Region on which to apply this command Name of the edge model being deleted

delete_interface_model

device= Device on which to apply this command
interface= Interface on which apply this command
name= Name of the interface model being deleted

delete node model

device= Device on which to apply this command region= Region on which to apply this command Name of the node model being deleted

edge_average_model

average_type=STRING, derivative=STRING)

device= Device on which to apply this command region= Region on which to apply this command

node_model= 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= The edge model name being created. If derivative is speci-

fied, the edge models created are edgeModel:derivativeModel@n0 edgeModel:derivativeModel@n1, which are the derivatives with re-

spect to the derivative model on each side of the edge

derivative= The node model of the variable for which the derivative is being

taken. The node model ${\tt nodeModel:derivativeModel}$ is used to cre-

ate the resulting edge models.

average_type= The node models on both sides of the edge are averaged together

to create one of the following types of averages.

"arithmetic" The edge model is the average of the node model on both sides

(default)

"geometric" The edge model is the square root of the product of the node model

evaluated on each side

"gradient"

The edge model is the gradient along the edge with respect to the

distance between the two nodes.

"negative_gradient" The edge model is the negative of the gradient along the edge

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

and the derivatives <code>ElectricField:Potential@n0</code> and <code>ElectricField:Potential@n1</code> are then created from

edge_from_node_model

device= Device on which to apply this command region= Region on which to apply this command

node_model= The node model from which we are creating the edge model

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

```
ds.edge_from_node_model(device=device, region=region, node_model="Potential")
```

edge_model

device= Device on which to apply this command Region= Region on which to apply this command Name of the edge model being created

equation= Equation used to describe the edge model being created

display_type= Option for output display in graphical viewer

"nodisplay" Data on edge will not be displayed

"scalar" Data on edge is a scalar quantity (default)

"vector" Data on edge is a vector quantity (deprecated)

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 element_from_edge_model command (page 26) to create components better suited for visualization. See *Chapter 10*, Visualization on page 65 for more information about creating data files for external visualization programs.

element_model

device= Device on which to apply this command region= Region on which to apply this command

name= Name of the element edge model being created

equation= Equation used to describe the element edge model being created

display_type= Option for output display in graphical viewer

"nodisplay" Data on edge will not be displayed

"scalar" Data on edge is a scalar quantity (default)

element_from_edge_model

device= Device on which to apply this command region= Region on which to apply this command

edge_model= The edge model from which we are creating the element model

derivative= The variable we are taking with respect to edge_model

For an edge model <code>emodel</code>, 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.

element_from_node_model

device= Device on which to apply this command region= Region on which to apply this command

node_model= The node model from which we are creating the edge model

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 be accessible as

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

where en0, and en1 refers 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 refers to the nodes on the nodes off the element edge on the tetrahedral element.

get_edge_model_list

```
ds.get_edge_model_list(device=STRING, region=STRING)

device= Device on which to apply this command
region= Region on which to apply this command
Returns a list of the edge models on the device region
```

get_edge_model_values

```
ds.get_edge_model_values(device=STRING, region=STRING, name=STRING)

device= Device on which to apply this command region= Region on which to apply this command name= Name of the edge model values being returned as a list
```

get_element_model_list

```
ds.get_edge_model_list(device=STRING, region=STRING)

device= Device on which to apply this command
    region= Region on which to apply this command
    Returns a list of the element edge models on the device region
```

get_element_model_values

get_interface_model_list

get_interface_model_values

name= Name of the interface model values being returned as a list

get_node_model_list

```
ds.get_node_model_list(device=STRING, region=STRING)

device= Device on which to apply this command
  region= Region on which to apply this command
  Returns a list of the node models on the device region
```

get_node_model_values

```
ds.get_node_model_values(device=STRING, region=STRING, name=STRING)

device= Device on which to apply this command region= Region on which to apply this command name= Name of the node model values being returned as a list
```

interface_model

```
ds.interface_model(device=STRING, interface=STRING, name=STRING, equation=STRING)

device= Device on which to apply this command interface= Interface on which apply this command equation= Equation used to describe the interface node model being created
```

interface normal model

```
ds.interface_normal_model(device=STRING, region=STRING, interface=STRING)

device= Device on which to apply this command

region= Region on which to apply this command
```

interface Interface on which apply this command 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.

node_model

device= Device on which to apply this command Region= name= Name of the node model being created

equation= Equation used to describe the node model being created

display_type= Option for output display in graphical viewer

"nodisplay" Data on node will not be displayed

"scalar" Data on node is a scalar quantity (default)

node_solution

ds.node_solution(device=STRING, region=STRING, name=STRING)

device= Device on which to apply this command region= Region on which to apply this command Name of the solution being created

print_node_values

device= Device on which to apply this command
region= Region on which to apply this command
name= Name of the node model values being printed to the screen

print_edge_values

device= Device on which to apply this command region= Region on which to apply this command

name= Name of the edge model values being printed to the screen

print_element_values

device= Device on which to apply this command region= Region on which to apply this command

name= Name of the element edge model values being printed to the screen

register_function

```
ds.register_function(name=STRING, nargs=STRING)
```

name= Name of the function

nargs= Number of arguments to the function

This command is used to register a new Python procedure for evaluation by SYMDIFF.

set_node_values

```
ds.set_node_values(device=STRING, region=STRING, name=STRING, init_from=STRING)

device= Device on which to apply this command region= Region on which to apply this command name= Name of the node model being initialized init_from= Node model we are using to initialize the node solution
```

symdiff

```
ds.symdiff(expr=STRING)
expr= Expression to send to SYMDIFF
```

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

vector_element_model

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

- \bullet emodel_x
- emodel_y
- emodel_z (3D only)

The primary use of these components are for visualization.

vector_gradient

```
ds.vector_gradient(device=STRING, region=STRING, node_model=STRING, calc_type=STRING)

device= Device on which to apply this command region= Region on which to apply this command

node_model= The node model from which we are creating the edge model calc_type= The node model from which we are creating the edge model Consider all nodes for calculating the gradient field (default)

"avoidzero" Do not take gradient at nodes where the node_model is zero
```

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 element_from_edge_model command (page 26) command can be used to create gradients for use in a simulation.

3.9 Geometry commands

get_device_list

```
ds.get_device_list()
```

Gets a list of devices on the simulation.

get_region_list

```
ds.get_region_list(device=STRING, contact=STRING, interface=STRING)
```

device= Device on which to apply this command

contact= If specified, gets the name of the region belonging to this contact on

the device (optional)

interface If specified, gets the name of the region belonging to this interface

on the device (optional)

get_contact_list

```
ds.get_contact_list(device=STRING)
```

device Device on which to apply this command

get_interface_list

```
ds.get_interface_list(device=STRING)
```

device Device on which to apply this command

Chapter 4

Model Parameters

Parameters can be set using the commands in *Section 4.4*, Material commands on page 34. There are two complementary formalisms for doing this.

4.1 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.

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

4.2 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.

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

4.3 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.

4.4 Material commands

get_dimension

```
ds.get_dimension (device=STRING)

device= Device on which to apply this command
```

get_parameter

name=

```
ds.get_parameter (device=STRING, region=STRING, name=STRING)

device= Device on which to apply this command
 region= Region on which to apply this command
```

Name of the parameter name being retrieved

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.

get_parameter_list

```
ds.get_parameter_list (device=STRING, region=STRING)

device= Device on which to apply this command
  region= Region on which to apply this command
```

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 get_parameter command (page 34), parameter names on the 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.

set_parameter

```
ds.set_parameter (device=STRING, region=STRING, name=STRING, value=STRING)

device= Device on which to apply this command

region= Region on which to apply this command

name= Name of the parameter name being retrieved

value= value to set for the parameter
```

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.

get_material

```
ds.get_material (device=STRING, region=STRING)

device= Device on which to apply this command region= Region on which to apply this command Returns the material for the specified region
```

set material

```
ds.set_material (device=STRING, region=STRING, material=STRING)

device= Device on which to apply this command

region= Region on which to apply this command

material= New material name

Sets the new material for a region.
```

create_db

```
ds.create_db (filename=STRING)
filename= filename to create for the db
```

open_db

```
ds.open_db (filename=STRING, permission=OPTION)

filename= filename to create for the db
permissions= permissions on the db
"readwrite" Open file for reading and writing
"readonly" Open file for read only (default)
```

close_db

```
ds.close_db()
```

Closes the database so that its entries are no longer available.

save_db

```
ds.save_db()
```

Saves any new or modified db entries to the database file.

add_db_entry

material= Material name requested. global refers to all regions whose mate-

rial does not have the parameter name specified

parameter= Parameter name

value = Value assigned for the parameter

unit= String describing the units for this parameter name description= Description of the parameter for this material type.

The save_db command is used to commit these added entries permanently to the database.

get_db_entry

ds.get_db_entry (material=STRING, parameter=STRING)

material= Material name parameter= Parameter name

This command returns a list containing the value, unit, and description for the requested material db entry.

Chapter 5

Circuits

5.1 Circuit elements

Circuit elements are manipulated using the commands in *Section 5.3*, Circuit commands on page 37. Using the circuit_element command (page 38) to add a circuit element will implicitly create the nodes being references.

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

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

5.2 Connecting devices

For devices to contribute current to an external circuit, the <code>contact_equation</code> command (page 19) should use the <code>circuit_node</code> 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 <code>circuit_node_alias</code> command (page 38) 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.

5.3 Circuit commands

Circuit commands are for adding circuit elements to the simulation.

add_circuit_node

name= Name of the circuit node being created
variable_update= update type for circuit variable

"default" Variable can be positive or negative

"log_damp" Variable update is damped

"positive" Solution update results in positive quantity

value= initial value

circuit alter

name= Name of the circuit element being modified param= parameter being modified (default *value*)

value = value for the parameter

circuit_element

name= Name of the circuit element being created. A prefix of "V" is for volt-

age source, "I" for current source, "R" for resistor, "L" for inductor, and

"C" for capacitor.

value= value for the default parameter of the circuit element

n1= circuit noden2= circuit node

acreal= real part of AC source for voltage acimag= imaginary part of AC source for voltage

circuit_node_alias

```
ds.circuit_node_alias (node=STRING, alias=STRING)
```

node= circuit node being aliased alias= alias for the circuit node

get_circuit_equation_number

ds.get_circuit_equation_number (node=STRING)

node= Circuit node

Returns the row number correspond to circuit node in a region. Values are only valid when during the course of a solve.

get_circuit_node_list

Gets the list of the nodes in the circuit.

```
get_circuit_node_list()
```

get_circuit_node_value

```
ds.get_circuit_node_value(solution=STRING, node=STRING)
```

solution= name of the solution. "dcop" is the name for the DC solution and is

the default

node= circuit node of interest

get_circuit_solution_list

```
ds.get_circuit_solution_list()
```

Gets the list of available circuit solutions.

set_circuit_node_value

solution= name of the solution. "dcop" is the name for the DC solution and is

the default

node= circuit node of interest

value= new value

Chapter 6

Meshing

6.1 1D mesher

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

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

The create_1d_mesh command (page 44) is first used to initialize the specification of a new mesh by the name specified with the mesh option. The add_1d_mesh_line command (page 44) is used to specify the end points of the 1D structure, as well as the location of points where the spacing changes. The tag is used to create reference labels used for specifying the contacts, interfaces and regions.

The add_1d_contact command (page 45), add_1d_interface command (page 45) and add_1d_region command (page 45) are used to specify the contacts, interfaces and regions for the device.

Once the meshing commands have been completed, the finalize_mesh command (page 44) is called to create a mesh structure and then create_device command (page 47) is used to create a device using the mesh.

6.2 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 add_2d_region command (page 46) 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.

```
ds.create_2d_mesh(mesh="cap")
ds.add_2d_mesh_line(mesh="cap", dir="y", pos=-0.001, ps=0.001)
ds.add_2d_mesh_line(mesh="cap", dir="x", pos=xmin, ps=0.1)
ds.add_2d_mesh_line(mesh="cap", dir="x", pos=xmax, ps=0.1)
ds.add_2d_mesh_line(mesh="cap", dir="y", pos=ymin, ps=0.1)
ds.add_2d_mesh_line(mesh="cap", dir="y", pos=ymax, ps=0.1)
ds.add_2d_mesh_line(mesh="cap", dir="y", pos=+1.001, ps=0.001)
ds.add_2d_region(mesh="cap", material="gas", region="gas1", yl=-.001, yh=0.0)
ds.add_2d_region(mesh="cap", material="gas", region="gas2", yl=1.0, yh=1.001)
ds.add_2d_region(mesh="cap", material="0xide", region="r0", xl=xmin, xh=xmax,
  yl=ymid1, yh=ymin)
ds.add_2d_region(mesh="cap", material="Silicon", region="r1", xl=xmin, xh=xmax,
  yl=ymid2, yh=ymid1)
ds.add_2d_region(mesh="cap", material="Silicon", region="r2", xl=xmin, xh=xmax,
 yl=ymid2, yh=ymax)
ds.add_2d_interface(mesh="cap", name="i0", region0="r0", region1="r1")
ds.add_2d_interface(mesh="cap", name="i1", region0="r1", region1="r2", xl=0, xh=1,
 yl=ymid2, yh=ymid2, bloat=1.0e-10)
ds.add_2d_contact(mesh="cap", name="top", region="r0", yl=ymin, yh=ymin, bloat=1.0e-10)
ds.add_2d_contact(mesh="cap", name="bot", region="r2", yl=ymax, yh=ymax, bloat=1.0e-10)
ds.finalize_mesh(mesh="cap")
ds.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 add_2d_contact command (page 46) or an interface using add_2d_interface command (page 46).

Once the meshing commands have been completed, the finalize_mesh command (page 44) is called to create a mesh structure and then create_device command (page 47) is used to create a device using the mesh.

6.3 Using an external mesher

The Gmsh meshing software (see Section 12.1.1, Gmsh on page 69) 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:

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

Once the meshing commands have been completed, the finalize_mesh command (page 44) is called to create a mesh structure and then create_device command (page 47) is used to create a device using the mesh.

6.4 Loading and saving results

The write_devices command (page 47) 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 "devsimdata" format is used for storing numerical information for use in other programs for analysis. The load_devices command (page 47) is then used to reload the device data for restarting the simulation.

6.5 Meshing commands

create_gmsh_mesh

```
ds.create_gmsh_mesh(mesh=STRING, file=STRING)
file= name of the Gmsh mesh file being read into DEVSIM
mesh= name of the mesh being generated
```

add_gmsh_contact

gmsh_name= physical group name in the Gmsh file
mesh= name of the mesh being generated
name= name of the contact begin created
region= region that the contact is attached to

add_gmsh_interface

gmsh_name= physical group name in the Gmsh file

mesh= name of the mesh being generated

name= name of the interface begin created

region0= first region that the interface is attached to

region1= second region that the interface is attached to

add_gmsh_region

gmsh_name= physical group name in the Gmsh file
mesh= name of the mesh being generated
region= name of the region begin created
material= material for the region being created

create_1d_mesh

```
ds.create_1d_mesh(mesh=STRING)
```

mesh= name of the 1D mesh being created

finalize mesh

```
ds.finalize_mesh(mesh=STRING)
```

mesh= Mesh to finalize

Finalize the 1D or 2D mesh so no additional mesh specifications can be added and devices can be created.

add_1d_mesh_line

mesh= Mesh to add the line to

tag= Text label for the position

pos= Position for the mesh point

ns= Spacing from this point in the negative direction (defaults to ps value)

ps= Spacing from this point in the positive direction

add 1d interface

```
ds.add_1d_mesh_interface mesh=STRING, tag=STRING, name=STRING)

mesh= Mesh to add the interface to

tag= Text label for the position to add the interface

name= Name for the interface being created
```

add_1d_contact

```
ds.add_1d_mesh_contact mesh=STRING, tag=STRING, name=STRING)
mesh= Mesh to add the contact to
tag= Text label for the position to add the contact
name= Name for the contact being created
```

ds.add_1d_region mesh=STRING, tag1=STRING, tag2=STRING,

add_1d_region

```
region=STRING, material=STRING)

mesh= Mesh to add the line to
tag1= Text label for the position bounding the region being added
tag2= Text label for the position bounding the region being added
region= Name for the region being created
material= Material for the region being created
```

create_2d_mesh

```
ds.create_2d_mesh mesh=STRING)
mesh= name of the 2D mesh being created
```

add 2d mesh line

add_2d_region

```
ds.add_2d_region mesh=STRING, region=STRING,
               material=STRING,
               x1=FLOAT, xh=FLOAT,
               yl=FLOAT, yh=FLOAT,
               bloat=FLOAT)
             Mesh to add the region to
 mesh=
 region=
             Name for the region being created
             Material for the region being created
 material=
             x position for corner of bounding box (default -MAXDOUBLE)
 xl =
             x position for corner of bounding box (default +MAXDOUBLE)
 xh=
             y position for corner of bounding box (default -MAXDOUBLE)
 yl=
             y position for corner of bounding box (default +MAXDOUBLE)
 yh=
             Extend bounding box by this amount when search for mesh to in-
 bloat=
             clude in region (default 1e-10)
```

add_2d_interface

```
ds.add_2d_interface mesh=STRING, name=STRING,
               region0=STRING, region1=STRING,
               xl=FLOAT, xh=FLOAT,
               yl=FLOAT, yh=FLOAT,
               bloat=FLOAT)
              Mesh to add the interface to
 mesh=
 interface=
              Name for the interface being created
              Name of the region included in the interface
 region0=
              Name of the region included in the interface
 region1=
 x1 =
              x position for corner of bounding box (default -MAXDOUBLE)
              x position for corner of bounding box (default +MAXDOUBLE)
 xh=
 yl=
              y position for corner of bounding box (default -MAXDOUBLE)
              y position for corner of bounding box (default +MAXDOUBLE)
 vh=
 bloat=
              Extend bounding box by this amount when search for mesh to in-
              clude in region (default 1e-10)
```

add_2d_contact

mesh= Mesh to add the contact to

contact= Name for the contact being created

region= Name of the region included in the contact

x1= x position for corner of bounding box (default -MAXDOUBLE)
xh= x position for corner of bounding box (default +MAXDOUBLE)
y1= y position for corner of bounding box (default -MAXDOUBLE)
yh= y position for corner of bounding box (default +MAXDOUBLE)
bloat= Extend bounding box by this amount when search for mesh to in-

clude in region (default 1e-10)

create_device

ds.create_device mesh=STRING, device=STRING)

mesh= name of the mesh being used to create a device

device= name of the device being created

load_devices

ds.load_devices(file=STRING)

file= name of the file to load the meshes from

write devices

ds.write_devices(file=STRING, device=STRING, type=OPTION)

file= name of the file to write the meshes to device= name of the device to write (optional)

type= format to use
"devsim" DEVSIM format

"devsim_data" DEVSIM output format with numerical data for all models

"floops" Floops format (for visualization in Postmini)
"tecplot" Tecplot format (for visualization in Tecplot)

"vtk" VTK format (for visualization in ParaView and VisIt)

Chapter 7

Solver

7.1 Solver

DEVSIM uses Newton methods to solve the system of PDE's. All of the analyses are performed using the solve command (page 51).

7.2 DC analysis

A DC analysis is performed using the solve command (page 51).

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

7.3 AC analysis

An AC analysis is performed using the solve command (page 51). A circuit voltage source is required to set the AC source.

7.4 Noise/Sensitivity analysis

An noise analysis is performed using the solve 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 solve command (page 51). If the equation begin solved is PotentialEquation, the names of the scalar impedance field is then:

- V1.I_PotentialEquation_real
- V1.I_PotentialEquation_imag

and the vector impedance fields evaluated on the nodes are

- V1.I_PotentialEquation_real_gradx
- V1.I_PotentialEquation_imag_gradx
- V1.I_PotentialEquation_real_grady (2D and 3D)
- V1.I_PotentialEquation_imag_grady (2D and 3D)
- V1.I_PotentialEquation_real_gradz (3D only)
- V1.I_PotentialEquation_imag_gradz (3D only)

7.5 Transient analysis

Transient analysis is performed using the solve command (page 51). DEVSIM supports timeintegration of the device PDE's. The three methods are supported are:

- BDF1
- TRBDF
- BDF2

7.6 Solver commands

get_contact_current

```
ds.get_contact_current(device=STRING, contact=STRING, equation=STRING)
```

```
device= Device on which to apply this command
contact= Contact on which to apply this command
equation= Name of the contact equation from which we are retrieving the current
```

get_contact_charge

```
ds.get_contact_charge(device=STRING, contact=STRING, equation=STRING)
```

```
device= Device on which to apply this command
contact= equation= Name of the contact equation from which we are retrieving the charge
```

solve

```
ds.solve(type=OPTION,
          solver_type=OPTION,
          absolute_error=FLOAT,
          relative_error=FLOAT,
          charge_error=FLOAT,
          maximum_iterations=INTEGER,
          frequency=FLOAT,
          output_node=STRING,
          gamma=FLOAT,
          tdelta=FLOAT)
                        type of solve being performed
 type=
  "dc"
                        DC steady state simulation
  "ac"
                         Small-signal AC simulation
  "noise"
                         Small-signal AC simulation
                         Perform DC steady state and keep calculate charge at initial time
  "transient_dc"
                        step
  "transient_bdf1"
                         Perform transient simulation using backward difference integration
  "transient_bdf2"
                         Perform transient simulation using backward difference integration
                         Perform transient simulation using trapezoidal integration
  "transient_tr"
 solver_type=
                        Linear solver type
                         Use LU factorization (default)
  "direct"
  "iterative"
                        Use iterative solver
                         Required update norm in the solve
 absolute_error=
                         Required relative update in the solve
 relative_error=
                         Relative error between projected and solved charge during transient
 charge_error=
                        simulation
                         Scaling factor for transient time step (default 1.0)
 gamma=
                        time step
 tdelta=
 maximum_iterations=
                        Maximum number of iterations in the DC solve
 frequency=
                        Frequency for small-signal AC simulation
```

Output circuit node for noise simulation

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

output_node=

Chapter 8

User Interface

8.1 Starting DEVSIM

Refer to *Chapter 11*, Installation *on page 67* for instructions on how to install DEVSIM. Once installed, DEVSIM may be invoked using the following command

devsim

for an interactive shell or

devsim filename.py

for batch mode where filename.py is the name of script being run. DEVSIM output is printed to the screen. To capture the output of the program, shell redirection commands may be used to direct the output to a file.

8.2 Python Language

8.2.1 Introduction

Python is the scripting language employed as the text interface to DEVSIM. Documentation and tutorials for the language are available from [2] A paper discussing the general benefits of using scripting languages may be found in [3].

8.2.2 DEVSIM commands

All of commands are in the ds namespace. In order to invoke a command, the command should be prefixed with ds., or the following may be placed at the beginning of the script:

from ds import *

For details concerning error handling, please see Section 8.4, Error handling on page 55.

8.2.3 Other packages

DEVSIM is able to load Python packages. It is important to note that binary extensions loaded into DEVSIM must be compatible with the operating system which it was compiled for. To load an extension, it is first necessary to provide the path as an environment variable, or at program run time.

For example, if the Python packages on your system are available in "/usr/share/tcltk", it is necessary to set the environment variable in "csh" as

```
setenv PYTHONPATH /usr/share/tcltk
or in "bash"
export PYTHONPATH=/usr/share/tcltk
In the Python script, this may be done using using the appropriate paths for your system
import sys
sys.path.append("/usr/share/tcltk")
```

Please see *Python* on page 69 for more information on obtaining a copy of Python for your computer's operating system.

8.2.4 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.

8.3 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. When reading a Unicode encoded script, the built in Python interpreter should be made aware of the encoding of the source encoding using this on the first or second line of the script

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

This option is only required on systems, such as Microsoft Windows, which do not default to this encoding. Care should be taken when using Unicode names for visualization using the tools in *Chapter 10*, Visualization on page 65, as this character set may not be supported.

8.4 Error handling

8.4.1 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 ds.error. It may be caught.

8.4.2 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 to DEVSIM LLC using the contact information in the front cover of this manual.

8.4.3 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.

8.4.4 Solver errors

When using the solve command (page 51), 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:

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

8.4.5 Verbosity

The set_parameter command (page 34) 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.

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

8.5 Parallelization

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

```
ds.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.

```
ds.set_parameter(name="threads_task_size", value=1024)
```

Chapter 9

SYMDIFF

9.1 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.

9.2 Syntax

9.2.1 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:

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

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

Table 9.1: Basic expressions involving unary, binary, and logical operators.

9.2.2 Basic expressions

In Table 9.1, 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 are 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.

Function	Description
B(exp1)	Bernoulli Function
dBdx(exp1)	derivative of Bernoulli function
derfcdx(exp1)	derivative of complementary error function
derfdx(exp1)	derivative error function
dFermidx(exp1)	derivative of Fermi Integral
dInvFermidx(exp1)	derivative of InvFermi Integral
<pre>dot2d(exp1x, exp1y, exp2x, exp2y)</pre>	exp1x*exp2x+exp1y *exp2y
erfc(exp1)	complementary error function
erf(exp1)	error function
exp(exp1)	exponent
Fermi(exp1)	Fermi Integral
ifelse(test, exp1, exp2)	if test is true, then evaluate exp1, otherwise exp2
if(test, exp)	if test is true, then evaluate exp, otherwise 0
InvFermi(exp1)	inverse of the Fermi Integral
log(exp1)	natural log
<pre>max(exp1, exp2)</pre>	maximum of the two arguments
min(exp1, exp2)	minimum of the two arguments
pow(exp1, exp2)	take exp1 to the power of exp2
sgn(exp1)	sign function
step(exp1)	unit step function
kahan3(exp1, exp2, exp3)	Extended precision addition of arguments
kahan4(exp1, exp2, exp3, exp4)	Extended precision addition of arguments

Table 9.2: Predefined Functions.

9.2.3 Functions

In Table 9.2 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.

Command	Description
diff(obj1, var)	Take derivative of obj1 with respect to variable
	var
expand(obj)	Expand out all multiplications into a sum of prod-
	ucts
help	Print description of commands
scale(obj)	Get constant factor
sign(obj)	Get sign as 1 or -1
<pre>simplify(obj)</pre>	Simplify as much as possible
<pre>subst(obj1,obj2,obj3)</pre>	substitute obj3 for obj2 into obj1
unscaledval(obj)	Get value without constant scaling
unsignedval(obj)	Get unsigned value
sum	sum of all the values over the entire region or in-
	terface

Table 9.3: Commands.

9.2.4 Commands

Commands are shown in Table 9.3. 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

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

Command	Description
clear(name)	Clears the name of a user function
<pre>declare(name(arg1, arg2,))</pre>	declare function name taking dummy arguments arg1, arg2, Derivatives assumed to be 0
<pre>define(name(arg1, arg2,), obj1, obj2,)</pre>	declare function name taking arguments arg1, arg2, having corresponding derivatives obj1, obj2,

Table 9.4: Commands for user functions.

9.2.5 User functions

Commands for specifying and manipulating user functions are listed in Table 9.4. 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 ${\tt f}$ which takes one argument.

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

The list after the function protoype 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:

```
> 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

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

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

```
> 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.

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

9.2.6 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.

```
> 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.

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

9.3 Invoking SYMDIFF from DEVSIM

9.3.1 Equation parser

The symdiff command (page 31) 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. Section 3.8, Model commands on page 21 presents commands which have the concepts of models. A ";" should be used to separate each statement.

This is a sample invocation from DEVSIM

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

9.3.2 Evaluating external math

The register_function command (page 30) 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:

```
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.

9.3.3 Models

When used withing the model commands discussed in *Section 3.8*, Model commands *on page 21*, 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.

Visualization

10.1 Introduction

DEVSIM is able to create files for visualization tools. Information about acquiring these tools are presented in *Chapter 12.1*, Third Party Software Availablilty on page 69.

10.2 Using Tecplot

The write_devices command (page 47) 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")
```

10.3 Using Postmini

The write_devices command (page 47) 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")
```

10.4 Using ParaView

The write_devices command (page 47) 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.

10.5 Using Vislt

Visit supports reading the Tecplot and ParaView formats. When using the vtk option on the write_devices command (page 47), a file with a visit filename extension is created to load the files created for ParaView.

10.6 DEVSIM

DEVSIM has several commands for getting information on the mesh. Those related to post processing are described in *Section 3.8*, Model commands on page 21 and *Section 3.9*, Geometry commands on page 32.

See Section 6.4, Loading and saving results on page 43 for information about loading and saving mesh information to a file.

Installation

11.1 Supported platforms

DEVSIM is has been compiled and tested on the platforms in Table 11.1. If you require a version of DEVSIM on a different software platform, please contact us using the information in the front cover of this manual.

11.2 Directory Structure

A devsim directory is created with the following sub directories.

bin contains the devsim binary

doc contains product documentation

lib contains runtime libraries

examples contains example scripts

11.3 Running DEVSIM

See Chapter 8, User Interface on page 53 for instructions on how to invoke DEVSIM.

Platform	Bits	OS Version
Microsoft Windows	32,64	Windows XP
		Windows 7
Linux	32,64	Ubuntu 8.04 (LTS)
		Ubuntu 10.04 (LTS)
		Ubuntu 12.04 (LTS)
		Centos 5 (Red Hat Enterprise 5 compatible)
Apple Mac OS X	32,64	Mac OS X 10.6 (Snow Leopard)

Table 11.1: Current platforms for DEVSIM.

Additional Information

12.1 Third Party Software Availablilty

12.1.1 Gmsh

Gmsh [4] is available from http://geuz.org/gmsh/.

12.1.2 ParaView

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

12.1.3 Postmini

Postmini is available from http://home.comcast.net/~john.faricelli/tcad.htm.

12.1.4 SQLite3

SQLite3 is the database engine used for the material database and is available from http://www.sqlite.com. It may be accessed from DEVSIM using

import sqlite3

12.1.5 **Python**

A Python distribution is not required for using DEVSIM, however additional packages from Python may be loaded into DEVSIM. Python is distributed with many operating system distributions. Additional information is available at http://www.python.org. It should be stressed that binary packages must be compatible with the Python distribution used by DEVSIM.

12.1.6 Tecplot

Tecplot is a visualization tool available from http://www.tecplot.com.

12.1.7 Vislt

Visit is a visualization tool available from https://wci.llnl.gov/codes/visit/.

12.2 Third Party Licenses

12.2.1 SuperLU

SuperLU [5] is used within DEVSIM and their copyright is reproduced here:

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Part II Examples

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 *Section 11.2*, Directory Structure *on page 67*.

The following example directories are contained in the distribution.

capacitance These are 1D and 2D capacitor simulations, using the internal mesher. A description of these examples is presented in *Chapter 14*, Capacitor on page 75.

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 *Chapter 15*, Diode on page 85.

bioapp1 This is a biosensor application.

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 Figure 13.1.

mobility This is an advanced example using electric field dependendent mobility models.

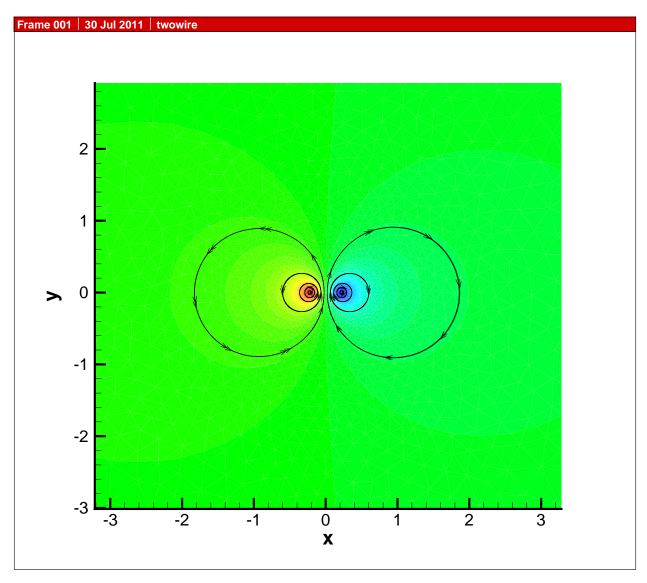


Figure 13.1: Simulation result for solving for the magnetic potential and field. The coloring is by the Z component of the magnetic potential, and the stream traces are for components of magnetic field.

Capacitor

14.1 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 Section 14.2, 1D Capacitor on page 75 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 Section 14.3, 2D Capacitor on page 79.

14.2 1D Capacitor

14.2.1 Equations

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

$$\varepsilon \nabla^2 \psi = 0 \tag{14.1}$$

and the contact boundary equations are

$$\psi_i - V_c = 0 \tag{14.2}$$

where ψ_i is the potential at the contact node and V_c is the applied voltage.

14.2.2 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 ds 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")
add_1d_contact (mesh="mesh1", name="contact2", tag="contact2")
add_1d_region (mesh="mesh1", material="Si", region=region, tag1="contact1", tag2="contact2")
finalize_mesh (mesh="mesh1")
create_device (mesh="mesh1", device=device)
```

14.2.3 Setting device parameters

In this section, we set the value of the permittivity to that of SiO₂.

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

14.2.4 Creating the models

Solving for the Potential, ψ , 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.

equation="EdgeInverseLength")

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

14.2.5 Contact boundary conditions

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

In this example, the contact bias is applied through parameters named <code>contact1_bias</code> and <code>contact2_bias</code>. When applying the boundary conditions through circuit nodes, models with respect to their names and their derivatives would be required.

14.2.6 Setting the boundary conditions

14.2.7 Running the simulation

We run the simulation and see the results.

```
capacitance > devsim cap1d.py
DEVSIM
Version: Beta 0.01
Copyright 2009-2013 Devsim LLC
contact2
(region: MyRegion)
(contact: contact1)
(contact: contact2)
Region "MyRegion" on device "MyDevice" has equations 0:10
Device "MyDevice" has equations 0:10
number of equations 11
Iteration: 0
 Device: "MyDevice" RelError: 1.00000e+00 AbsError: 1.00000e+00
   Region: "MyRegion" RelError: 1.00000e+00 AbsError: 1.00000e+00
     Equation: "PotentialEquation" RelError: 1.00000e+00 AbsError: 1.00000e+00
Iteration: 1
 Device: "MyDevice" RelError: 2.77924e-16 AbsError: 1.12632e-16
   Region: "MyRegion" RelError: 2.77924e-16 AbsError: 1.12632e-16
     Equation: "PotentialEquation" RelError: 2.77924e-16 AbsError: 1.12632e-16
contact: contact1 charge: 3.45150e-13
contact: contact2 charge: -3.45150e-13
```

Which corresponds to our expected result of 3.451510^{-13} F/cm² for a homogenous capacitor.

14.3 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.

14.4 Defining the mesh

```
from ds 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
v3 = 0.8
y4 = 0.9
vmax=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", yl=y1, yh=y2, xl=x1, xh=x4)
add_2d_contact(mesh=device, name="top", region="air", yl=y3, yh=y4, xl=x2, xh=x3)
finalize_mesh(mesh=device)
create_device(mesh=device, device=device)
```

14.5 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
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
edge_model(device=device, region=region, name="ElectricField",
                 equation="(Potential@n0 - Potential@n1)*EdgeInverseLength")
edge_model(device=device, region=region, name="ElectricField:Potential@n0",
                 equation="EdgeInverseLength")
edge_model(device=device, region=region, name="ElectricField:Potential@n1",
                 equation="-EdgeInverseLength")
###
### Model the D Field
###
edge_model(device=device, region=region, name="DField",
           equation="Permittivity*ElectricField")
edge_model(device=device, region=region, name="DField:Potential@n0",
           equation="diff(Permittivity*ElectricField, Potential@n0)")
edge_model(device=device, region=region, name="DField:Potential@n1",
           equation="-DField:Potential@n0")
```

Create the bulk equation

```
equation(device=device, region=region, name="PotentialEquation", variable_name="Potential",
    edge_model="DField", variable_update="default")
### Contact models and equations
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")
###
### Set the contact
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 100 -solver_type iterativ
solve(type="dc", absolute_error=1.0, relative_error=1e-10, maximum_iterations=30, solver_type="direct")
```

14.6 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.

```
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")
```

14.7 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: 1.00000e+00
Iteration: 1
 Device: "MyDevice" RelError: 1.25144e-12 AbsError: 1.73395e-13
   Region: "air" RelError: 1.25144e-12 AbsError: 1.73395e-13
     Equation: "PotentialEquation" RelError: 1.25144e-12 AbsError: 1.73395e-13
3.35017166004e-12
-3.35017166004e-12
```

A visualization of the results is shown in Figure 14.1.

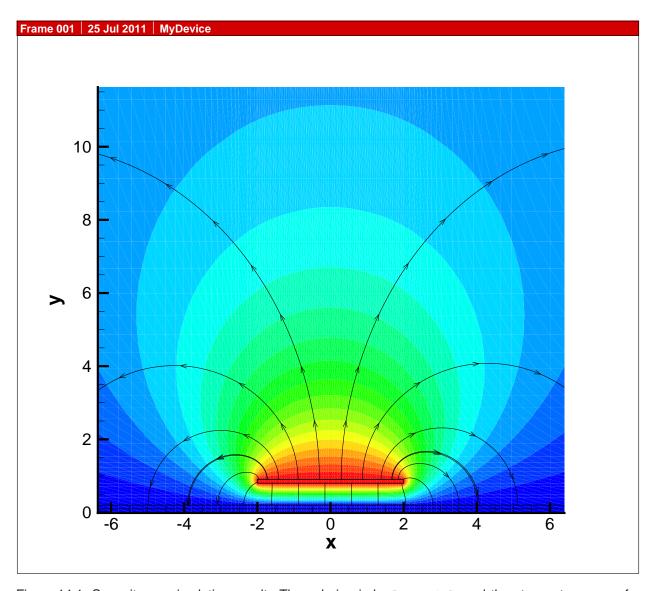


Figure 14.1: Capacitance simulation result. The coloring is by Potential, and the stream traces are for components of ElectricField.

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 [6].

15.1 1D diode

15.1.1 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 15.1. The python_packages must be in your path, and may be set using the methods described in *Section 8.2.3*, Other packages on page 54. The example files in the DEVSIM distribution set the path properly when loading modules.

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

```
from ds import *
from simple_physics import *
```

15.1.2 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")
    add_1d_contact (mesh="dio", name="bot", tag="bot")
    add_1d_region (mesh="dio", material="Si", region=region, tag1="top", tag2="bot")
    finalize_mesh(mesh="dio", device=device)
```

model_create	Creation of models and their derivatives
ramp	Ramping bias and automatic stepping
simple_dd	Functions for calculating bulk electron and hole
	current
simple_physics	Functions for setting up device physics

Table 15.1: Python package files.

```
device="MyDevice"
region="MyRegion"
createMesh(device, region)
```

15.2 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
solve(type="dc", absolute_error=1.0, relative_error=1e-12, maximum_iterations=30)
####
#### drift diffusion solution variables
####
CreateSolution(device, region, "Electrons")
CreateSolution(device, region, "Holes")
####
#### create initial guess from dc only solution
####
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
CreateSiliconDriftDiffusion(device, region)
for i in get_contact_list(device=device):
 CreateSiliconDriftDiffusionAtContact(device, region, i)
###
### Drift diffusion simulation at equilibrium
solve(type="dc", absolute_error=1e10, relative_error=1e-10, maximum_iterations=30)
#### Ramp the bias to 0.5 Volts
####
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
write_devices(file="diode_1d.dat", type="tecplot")
```

15.2.1 Plotting the result

A plot showing the doping profile and carrier densities are shown in Figure 15.1. The potential and electric field distribution is shown in Figure 15.2. The current distributions are shown in Figure 15.3.

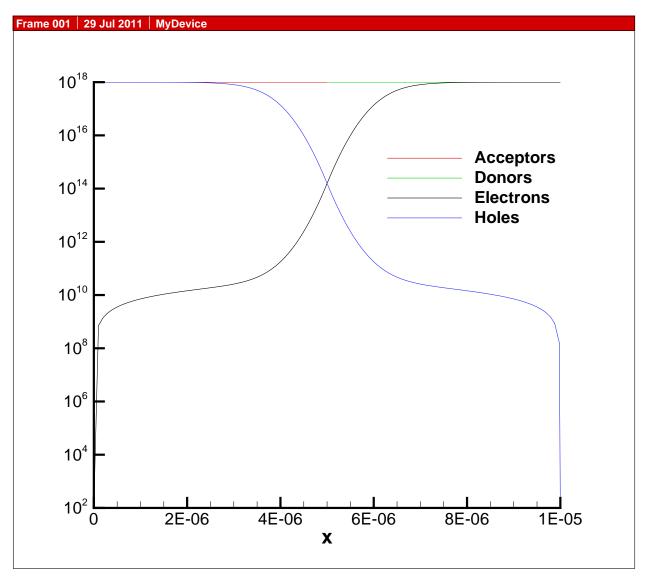


Figure 15.1: Carrier density versus position in 1D diode.

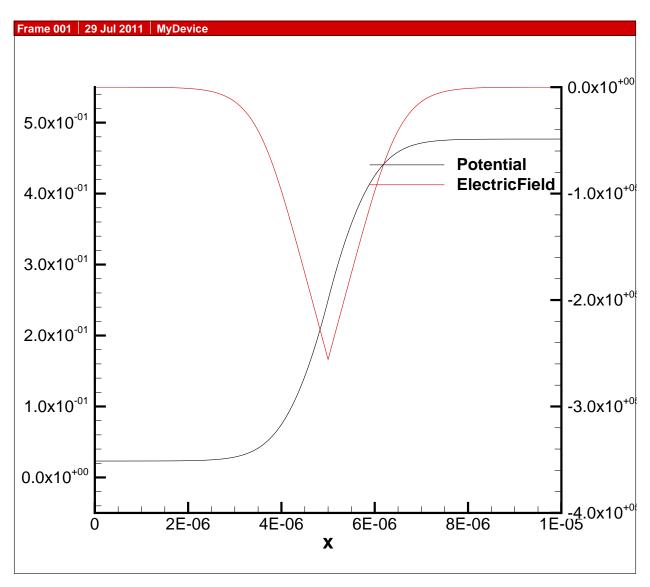


Figure 15.2: Potential and electric field versus position in 1D diode.

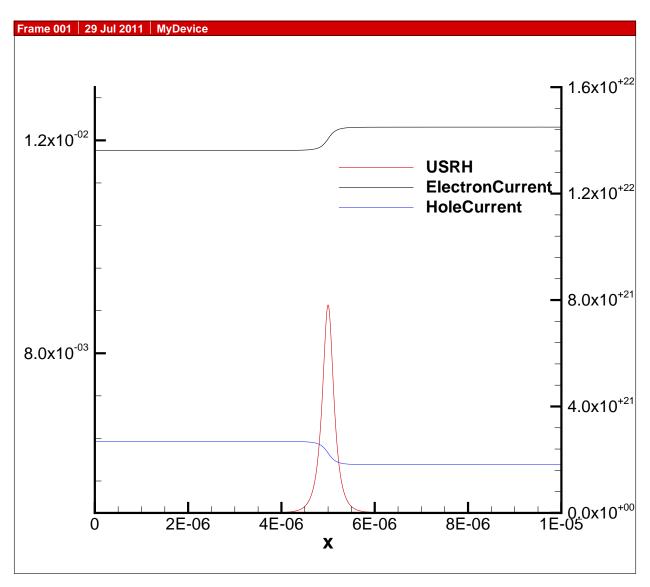


Figure 15.3: Electron and hole current and recombination.

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