Sentaurus™ Mesh User Guide

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SYNOPSYS®

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About This Guide

The Synopsys Sentaurus™ Mesh tool is a mesh generator that incorporates different mesh generation engines: an axis-aligned mesh generator, an offsetting mesh generator, and a tensor-product mesh generator that produces rectangular or hexahedral elements. Sentaurus Mesh is designed to be used in a wide range of simulators, including the Synopsys TCAD products Sentaurus Device, Sentaurus Process, Sentaurus Device Electromagnetic Wave Solver, and Sentaurus Interconnect. Local mesh refinement is performed using the doping and refinement information in the mesh command file.

Related Publications

For additional information, see:

- The TCAD Sentaurus release notes, available on the Synopsys SolvNet® support site (see Accessing SolvNet on page viii).
- Documentation available on SolvNet at https://solvnet.synopsys.com/DocsOnWeb.

Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
Blue text	Identifies a cross-reference (only on the screen).
Bold text	Identifies a selectable icon, button, menu, or tab. It also indicates the name of a field or an option.
`Courier font`	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.
Italicized text	Used for emphasis, the titles of books and journals, and non-English words. It also identifies components of an equation or a formula, a placeholder, or an identifier.

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- support-tcad-ap@synopsys.com from within Asia Pacific (China, Taiwan, Singapore, Malaysia, India, Australia).
- support-tcad-kr@synopsys.com from Korea.
- support-tcad-jp@synopsys.com from Japan.

CHAPTER 1 Introduction to Sentaurus Mesh

This chapter describes how to start Sentaurus Mesh and provides a general explanation of its functionality.

Overview

Sentaurus Mesh is a suite of tools that produce finite-element meshes for use in applications such as semiconductor device simulations, process simulations, and electromagnetic simulations. It has three mesh generation engines: an axis-aligned mesh generator, an offsetting mesh generator, and a tensor-product mesh generator. Sentaurus Mesh also provides a set of tools that perform operations on boundary representations and meshes.

The axis-aligned and offsetting mesh generators produce Delaunay meshes, which are suitable for use in Sentaurus Device and Sentaurus Process. In one dimension, the meshes contain segments only. In two dimensions, the meshes contain triangles only, while in three dimensions, the meshes comprise tetrahedra. For information about the algorithm used to generate Delaunay meshes, see Chapter 6 on page 107.

The offsetting mesh generator can produce layered meshes in two and three dimensions. The layers are located at the device interfaces and follow the contours of the interface. They can be combined with axis-aligned elements to produce high-quality meshes for nonplanar structures. As such, the offsetting mesh generator is a superset of the axis-aligned mesh generator, where layering takes precedence over axis-aligned mesh generation.

The tensor-product mesh generator is currently intended to generate meshes for Sentaurus Device Electromagnetic Wave Solver and for some applications in Sentaurus Device. The meshes contain rectangular elements in two dimensions and cuboid elements in three dimensions.

Sentaurus Mesh reads the input geometry from a boundary file stored in the TDR format with the `_bnd.tdr` file extension. Some TDR files from Sentaurus Process and Sentaurus Interconnect with the `_fps.tdr` and `_sis.tdr` file extensions, respectively, contain two geometry objects: one for the volumetric data and one for the boundary representation. Sentaurus Mesh reads the boundary object in these TDR files, but it ignores other geometry objects.

See Sentaurus™ Data Explorer User Guide, Appendix B on page 119 for details about the TDR file structure.

Impurity concentrations and user-required element sizes can be described using a mesh command file. The grid can be adapted to analytic profiles generated by Sentaurus Structure Editor or profiles generated by Sentaurus Process. (All references to concentrations in this document imply ‘active’ or ‘substitutional’ concentrations, since calculations in Sentaurus Device use concentrations in this form.)

The required point density is obtained by refining the elements in an anisotropic way. Therefore, unnecessary point propagation due to quadtrees, octrees, or tensor-product grid techniques is avoided.

A delaunization process allows Sentaurus Mesh to obtain high-quality conforming Delaunay grids, suitable for control volume discretization methods that are used in device simulation. For more information, refer to the literature [1][2][3][4][5].

The output of Sentaurus Mesh depends on the mesh generation engine used. The axis-aligned and offsetting mesh generators always produce a TDR unstructured mesh; the tensor-product mesh generator will select the type of mesh depending on the target application.

Applications of Different Mesh Generators

The choice of which mesh generator to use for a particular application depends largely on the geometry of the device.

For devices where the most important surfaces are axis aligned, the recommendation is to use the axis-aligned mesh generator, since it produces the highest quality elements with minimal node count for such devices.

For devices where the main surfaces are nonaxis-aligned or curved (for example, a MOS-type structure where the channel is nonplanar), the recommendation is to use the offsetting mesh generator, since it produce meshes containing layers that better conform to the curved surfaces, thereby reducing the number of elements in the final mesh (see Offsetting Section on page 37).

For electromagnetic simulations using Sentaurus Device Electromagnetic Wave Solver, use the tensor-product mesh generator.

Starting Sentaurus Mesh

In Sentaurus Mesh, a mesh is created from two input files, namely, the boundary file and the command file. If the input project is called `project_name`, a mesh can be created using the command:

```
snmesh [options] project_name
```

Sentaurus Mesh automatically adds the extensions `_bnd.tdr` and `.cmd` to the base name `project_name`. Sentaurus Mesh creates the output file `project_name_msh.tdr` that contains mesh geometry information and doping information. Another file, `project_name_msh.log`, is created and is used as the log file for the mesh generation.

Command-Line Options

The binary of Sentaurus Mesh is `snmesh`. It is executed using the syntax:

```
snmesh [options] <command_file_name>
```

Table 1 Command-line options available for Sentaurus Mesh

Option	Description
`-backcompat <release>`	Changes the behavior of the mesh generation and solid-modeling algorithms and variable defaults to those of a specified previous release. For example: `-backcompat M-2016.12-SP1`
`-h`	Displays help information.
`-v`	Displays version information only.

References

[1] L. Villablanca, *Mesh Generation Algorithms for Three-Dimensional Semiconductor Process Simulation*, Series in Microelectronics, vol. 97, Konstanz, Germany: Hartung-Gorre, 2000.

[2] P. Conti, M. Tomizawa, and A. Yoshii, “Generation of Oriented Three-Dimensional Delaunay Grids Suitable for the Control Volume Integration Method,” *International Journal for Numerical Methods in Engineering*, vol. 37, no. 19, pp. 3211–3227, 1994.

[3] G. Garretón *et al.*, “A New Approach for 2-D Mesh Generation for Complex Device Structures,” in *International Workshop on Numerical Modeling of Processes and Devices for Integrated Circuits (NUPAD V)*, Honolulu, HI, USA, pp. 159–162, June 1994.

[4] G. Garretón *et al*., "Unified Grid Generation and Adaptation for Device Simulation," in *Simulation of Semiconductor Devices and Processes (SISDEP)*, vol. 6, Erlangen, Germany, pp. 468–471, September 1995.

[5] G. Heiser, *Design and Implementation of a Three-Dimensional General Purpose Semiconductor Device Simulator*, Series in Microelectronics, vol. 13, Konstanz, Germany: Hartung-Gorre, 1991.

CHAPTER 2 Command File

This chapter describes the sections of the command file of Sentaurus Mesh.

Overview

In the command file (`.cmd`), you can specify different parameters for the generation of a mesh as follows:

- Sections are delimited by opening and closing braces.
- Only one keyword must be specified per line.
- Keywords used in the command file are not case sensitive.
- Strings are enclosed in double quotation marks.
- Comments start with `*` or `#`.

Different types of information can be given in the command file. You can specify refinement information, doping profile information, and control parameters for the different mesh generators and tools provided in Sentaurus Mesh.

Refinement information is required to control mesh generation according to user requirements (local element size). This information is specified in the `Definitions` section. Profile information is required to define the fields, for example, doping profiles, which are used in grid adaptation. Doping profiles can be specified with different types of information:

- External simulation results
- Constant data
- Analytic formulas and predefined functions describing a profile

The command file has the following sections:

- The command file can start with an optional title statement, which consists of the `Title` keyword followed by a string in double quotation marks. By default, `Title ""` is used.
- `IOControls` specifies an explicit input file containing the structure and an output file to which the generated mesh will be saved.
- `Definitions` defines the sets of refinement parameters and profile definitions to be used in the `Placements` section. These sets are referred to using their unique *reference name*.
- `Placements` defines instances of the definitions given in the `Definitions` section, placed with respect to the current device.

- `Interpolate` controls data interpolation.
- `AxisAligned` controls the axis-aligned mesh generator.
- `Offsetting` controls the offsetting mesh generator.
- `Delaunizer` controls the behavior of the delaunizer in Sentaurus Mesh.
- `Tensor` controls the tensor-product mesh generator.
- `Tools` specifies additional meshing utilities available in Sentaurus Mesh.
- `QualityReport` specifies the mesh quality statistics to be reported and the limits for the mesh quality criteria.

The syntax of the command file is:

```
Title ""
IOControls {input/output information}
Definitions {defining information}
Placements {placing information}
Interpolate {data interpolation information}
AxisAligned {axis alignment information}
Offsetting {offsetting information}
Delaunizer {delaunizer information}
Tensor {tensor information}
Tools {tools information}
QualityReport {mesh quality information}
```

The different sections of the command file of Sentaurus Mesh are described in the next sections.

IOControls Section

The `IOControls` section is used to specify the names of input files describing the structure and the name of the output file with the generated result. The input and boundary files can contain either a boundary or a mesh in TDR format.

You can use the `EnableOffset`, `EnableSections`, `EnableTensor`, and `EnableTools` options to enable different algorithms based on the contents of the command file. The result after enabling unrelated sections in the command file is undefined.

The syntax of this section is:

```
IOControls {
   EnableEMW
   EnableOffset
   EnableSections
   EnableTensor
```

```
    EnableTools
    inputFile = "string"
    numThreads = integer
    outputFile = "string"
    useDFISEcoordinates
    useUCScoordinates
    verbosity = 0 | 1 | 2 | 3
}
```

where (default values are given in parentheses if applicable):

`EnableEMW`

Generates meshes suitable for Sentaurus Device Electromagnetic Wave Solver (EMW) applications using the tensor-product mesh generator (see EMW Subsection for Computing Cell Size Automatically on page 48).

`EnableOffset`

Enables the `Offsetting` section of the command file and the offsetting mesh generator (see Offsetting Section on page 37).

`EnableSections`

Parses the command file and activates the mesh generators associated with the sections present in the command file. If the command file contains the `AxisAligned`, `Tools`, `Tensor`, or `Offsetting` sections, the `EnableSections` option activates automatically the corresponding mesh generators.

`EnableTensor`

Enables the tensor-product mesh generator (see Tensor Section on page 43).

`EnableTools`

Enables the operations that can be specified in the `Tools` section (see Tools Section on page 53).

`inputFile`

The name of the default input file is based on the name of the command file. If an input file is specified, it is used as the input file instead of the default input file based on the name of the command file.

`numThreads (1)`

Sets the number of threads to be used by the mesh generators (axis-aligned, offsetting, and tensor-product).

`outputFile`

Specifies the name of the output file.

`useDFISEcoordinates`

Converts all coordinates to the DF–ISE coordinate system (except the coordinates from the command file).

`useUCScoordinates`

Uses the unified coordinate system (UCS). With the exception of the command file, the coordinates from all files read by Sentaurus Mesh are converted to the UCS.

`verbosity`

Sets the verbosity level of the output messages. At level 0, only basic messages are displayed. At level 3, all messages are displayed.

Definitions Section

The `Definitions` section is composed of sets of refinement and profile subsections. Each subsection consists of a reference name, an opening brace, the specification of parameters, and a closing brace.

The order of definitions in the `Definitions` section is not important since these definitions are used as references in the `Placements` section.

The syntax of this section is:

```
Definitions {
   Refinement "reference name" {parameters}
   Multibox "reference name" {parameters}
   Constant "reference name" {parameters}
   AnalyticalProfile "reference name" {parameters}
   SubMesh "reference name" {parameters}
   Particle "reference name" {parameters}
   ...
}
```

Defining Refinement Regions

The syntax to define a refinement region is:

```
Refinement "reference name" {
   MaxElementSize = value | vector
   MinElementSize = value | vector
   RefineFunction = MaxGradient(parameters) | MaxTransDifference(parameters) |
                    MaxInterval(parameters) | MaxLengthInterface(parameters)
}
```

where (default values are given in parentheses if applicable):

`MaxElementSize (1)`

Controls the maximum size of the grid elements (you also can use its abbreviation `MaxElemSize`). A real number or a vector $\vec{x} = [x_1, \ldots, x_d]$ can be specified, where d is the dimension and x_d represents the maximum edge lengths along the coordinate axes. A vector can be used to refine nonisotropically. Only values greater than zero are considered.

`MinElementSize (0.02)`

Controls the minimum size of the grid elements (you also can use its abbreviation `MinElemSize`). A real number or a vector $\vec{x} = [x_1, \ldots, x_d]$ can be specified, where x_d represents the minimum edge lengths along the coordinate axes. Grid elements can be refined in one direction if their edge length in that direction is greater than the specified value. Only values greater than zero are considered.

`RefineFunction (MaxTransDifference)`

Different functions can be used to select grid elements for refinement:

- `MaxGradient` (or use its abbreviation `MaxGrad`): The gradient of a profile (`Variable`) in the element is evaluated. If the gradient is greater than `Value` and the edge lengths are large enough, the element is refined. The syntax is:

  ```
  RefineFunction = MaxGradient(Variable = "Dataset name",
     Value = value | vector | tensor)
  ```

- `MaxTransDifference` (or use its abbreviation `MaxTransDiff`): The maximum difference of the transformed values of a profile at the vertices of the element is evaluated. If the difference is greater than `Value` and the edge lengths are large enough, the element is refined. The syntax is:

  ```
  RefineFunction = MaxTransDifference(Variable = "Dataset name",
     Value = value | vector | tensor)
  ```

The transformation applied to the values used in the refinement functions (linear, logarithmic, arsinh) is defined in the `datexcodes.txt` file for each `Variable` (see Utilities User Guide, Variables on page 2).

`RefineFunction` can be repeated for different variables in the same `Refinement` section. If `Variable` is not defined, the default is `"DopingConcentration"`. If `Value` is not specified, it defaults to 1; however, no `RefineFunction` is assigned by default.

`Variable` defines the dataset used to adapt the grid. The grid can be adapted according to species or any type of variable defined in the output file. The values are computed from the analytic formulas, constant data, and external simulation results defined in the command file. Therefore, the name of a variable must match the name of a variable stored in the output file. The variable name must be enclosed in double quotation marks.

The parameter `Value` can be used to refine scalar, vector, or tensor variables.

To refine on a vector variable, use a vector of values, one per direction. For example, in two dimensions, you can refine on `ElectricField` as follows:

```
RefineFunction = MaxTransDiff(Variable = "ElectricField",
   Value = (100,100) )
```

To refine on a tensor variable, use an array of 9 elements where each component is represented like this: `(xx xy xz yx yy yz zx zy zz)`. Alternatively, if the tensor field has symmetric components, you can use a 6-element array like this: `{xx xy yy yz zx zz}`. For example, you can refine on `Stress` as follows:

```
RefineFunction = MaxTransDiff(Variable = "Stress",
   Value = (1e10 2e10 1e10 1e8 1e10 1e10 2e10 1e10 1e8) )
```

The refinement is applied independently to each component of the vectors and tensors.

- `MaxInterval`: This function analyzes each edge in a refinement tree cell and refines the edge if the data values at the endpoints overlap a given interval and the edge is longer than the maximum edge length defined on the interval. The syntax is:

  ```
  RefineFunction = MaxInterval(Variable = "Dataset name",
     cmin = value | vector | tensor, cmax= value | vector | tensor,
     targetLength = value, scaling = value, rolloff)
  ```

  If the values at the edge endpoints overlap the range given by `cmin` and `cmax`, the algorithm checks only whether the edge length is shorter than the `targetLength` value. If this happens, the edge will be split.

  When the edge is outside the value range, and the `rolloff` variable is true, the tool adjusts `targetLength` to have a smooth transition into the coarser areas. To do this, the tool applies the following formula:

  ```
  targetLengthOutside = targetLength*(1 + log(Ca) - log(Cb))^2 * scaling
  ```

where `Ca` and `Cb` are the variable values at the endpoints of the edge.

- `MaxLengthInterface` (or use its abbreviation `MaxLenInt`): This function produces refinement at the interfaces. The syntax is:

  ```
  RefineFunction = MaxLengthInterface(Interface("Material1","Material2"),
     Value = value, Factor = value, DoubleSide, UseRegionNames)
  ```

  `RefineFunction` can be repeated for different interfaces in the same `Refinement` section.

  The material specified in the `Interface` statement must be a valid DATEX material. The first material indicates the side of the interface on which the refinement is performed. To apply the refinement to both sides of the interface, specify the `DoubleSide` option.

  By default, interfaces are defined by a pair of materials. However, if the option `UseRegionNames` is used, the interface is interpreted as a regionwise specification.

  The material `"All"` can be used to specify all interfaces of a given material and an empty string can be used to specify outer interfaces. In addition, the second argument in an interface specification can be a contact indicated by either the string `"Contact"` or the name of the contact (if `UseRegionNames` is specified).

  If `Interface` is not defined, no interface will be refined. If `Value` is not specified, it defaults to 1. The `Factor` parameter must be a number greater than or equal to 1. If `Factor` is not defined, it defaults to a huge number, so only one layer is produced.

Defining Multibox Regions

NOTE Using the `Multibox` subsection is no longer recommended. Instead, use interface refinement with `MaxLengthInterface` (see Performing Interface Refinement on page 81).

A multibox is a special refinement box that specifies a graded refinement along the x-, y-, or z-direction. You can specify the required minimum and maximum element sizes, and an additional refinement ratio in all directions. The created mesh is graded using the specified ratios (also observing the minimum and maximum element sizes). The syntax to define a multibox refinement region is:

```
Multibox "reference name" {
   MaxElementSize = value | vector
   MinElementSize = value | vector
   Ratio = (ratio_width, ratio_height, ratio_depth)
}
```

where:

- `MaxElementSize` and `MinElementSize` are the same as described in Defining Refinement Regions on page 9.
- `Ratio` controls the grading of the element sizes:
  - *`ratio_width`* is the grading factor in the x-direction.
  - *`ratio_height`* is the grading factor in the y-direction.
  - *`ratio_depth`* is the grading factor in the z-direction (3D only).

Defining Constant Profiles

The syntax to define a constant profile is:

```
Constant "reference name" {
   Species = "string"
   Value = value
}
```

where:

`Species`

Specifies the species or variables for the constant profile.

`Value`

Specifies the value of the constant profile.

Defining Analytic Profiles

Profiles can be defined using simple analytic expressions, which have two components. The first component `Function` represents the values along a direction defined as the normal direction of the `ReferenceElement`. This is the *primary direction*. These values are smoothed along the direction perpendicular to the normal, or *lateral direction*, using the second component `LateralFunction`.

These expressions can be of the following types:

- Predefined functions: Gaussian and error function
- One-dimensional external profile
- Your own function (using the general function evaluator)

The formulas used for these analytic profiles are described in Appendix A on page 111.

The syntax to define an analytic profile is (instead of `AnalyticalProfile`, you can use its abbreviation `AnaProf`):

```
AnalyticalProfile "reference name" {
   Species = "string"
   Function = Gauss(primary parameters) | Erf(primary parameters) |
              subMesh1D(primary parameters) |
              Eval(primary parameters) | General(primary parameters)
   LateralFunction = Gauss(lateral parameters) | Erf(lateral parameters) |
                     Eval(lateral parameters)
}
```

where:

`Species`

Specifies the species for the analytic profile.

`Function`

Indicates the type of function and the parameters used along the primary direction, the direction normal to the `ReferenceElement`.

`LateralFunction`

Defines the lateral component of the analytic profile (you also can use its abbreviation `LatFunc`). A Gaussian function, an error function, or a general analytic function can be specified using the following lateral parameters:

```
LateralFunction = Gauss(Factor = value)
LateralFunction = Gauss(StandardDeviation = value)
LateralFunction = Gauss(Length = value)
LatFunc = Erf(Factor = value)
LatFunc = Erf(Length = value)
LatFunc = Eval(init = "..." function = "...")
```

NOTE The default `LateralFunction` is the error function `Erf`.

NOTE If you use `General` to specify the analytic profile, there is no separate `LateralFunction` since the definition of the analytic profile using `General` includes both the primary and the lateral directions in its formulation.

Specifying a Gaussian Function

A Gaussian function can be specified with the following primary parameters:

```
Function = Gauss(PeakPosition = value, PeakValue = value,
           StandardDeviation = value)
Function = Gauss(PeakPosition = value, Dose = value, StdDev = value)
Function = Gauss(PeakPosition = value, PeakValue = value, Length = value)
Function = Gauss(PeakPosition = value, Dose = value, Length = value)
Function = Gauss(PeakPosition = value, PeakValue = value,
           ValueAtDepth = value, Depth = value)
Function = Gauss(PeakPos = value, Dose = value, ValAtDepth = value,
           Depth = value)
```

By default, `PeakPosition=0`. There are no default values for the other parameters.

If `Function=Gauss`, `Factor=0.8` in `LateralFunction` by default.

Some parameters have abbreviations (provided in parentheses) you can use, including: `StandardDeviation` (`StdDev`), `PeakPosition` (`PeakPos`), `PeakValue` (`PeakVal`), and `ValueAtDepth` (`ValAtDepth`).

Specifying an Error Function

An error function can be specified with the following primary parameters:

```
Function = Erf(SymmetryPosition = value, MaxValue = value, Length = value)
Function = Erf(SymmetryPosition = value, Dose = value, Length = value)
Function = Erf(SymPos = value, MaxVal = value, ValAtDepth = value,
           Depth = value)
Function = Erf(SymPos = value, Dose = value, ValAtDepth = value,
           Depth = value)
```

By default, `SymmetryPosition=0`.

If `Function=Erf`, `Factor=0.8` in `LateralFunction` by default.

Some parameters have abbreviations (provided in parentheses) you can use, including: `SymmetryPosition` (`SymPos`) and `MaxValue` (`MaxVal`).

Specifying a 1D External Profile

To specify a 1D external profile, the syntax is:

```
Function = subMesh1D(Datafile = "string", DataScale = value,
           Scale = value, Range = line [(x1), (x2)])
```

The `Datafile` parameter specifies a file in XGRAPH format, which consists of a title enclosed in double quotation marks and a list of `"x y"` values. More than one profile can be included in `Datafile`.

The `DataScale` parameter scales the data values contained in the data file. Each input value is multiplied by the `DataScale` factor. By default, `DataScale=1`.

The `Scale` parameter scales the coordinate values from the file. By default, `Scale=1`.

The optional `Range` parameter selects a range of values from the file. The keywords `x1` and `x2` must be given in the file coordinate system. `Range` is applied to all profiles inside the file. By default, the entire data range is selected.

If `Function=subMesh1D`, `StandardDeviation=0.8` in `LateralFunction` by default.

Using the General Function Evaluator

The general function evaluator can be used in either of two ways:

- Using `Eval`: A user-specified analytic function in the primary direction (normal to the reference window) and a separate decay function (Gaussian, error function, or a user-defined function with `Eval`) in the lateral direction. The syntax is:

```
AnalyticalProfile "reference name" {
   Function = Eval(init = "string", function = "string", value = value)
   LateralFunction = Eval(init = "string", function = "string")
}
```

- Using `General`: A user-defined function specified directly in device coordinates. There is no concept of primary and lateral directions because the `General` function is specified directly as a function of the x-, y-, and z-direction. The syntax is:

```
AnalyticalProfile "reference name" {
   Function = General(init = "string", function = "string", value = value)
}
```

NOTE `General` does not require `LateralFunction` since the `General` function is evaluated directly in all device coordinates.

Both the `Eval` and `General` functions use the same syntax for the primary parameters. The difference is that `General` uses spatial coordinates and `Eval` uses coordinates that are measured in the primary or lateral profile direction when used to define the primary or lateral profile, respectively.

The keywords `init`, `function`, and `value` correspond to the initialization formula, the evaluation formula, and the default value (in the case of a failed formula evaluation at a data point) (for the use of `General` functions, see Using Analytic Functions for Refinement I on page 89):

`init`

Specifies a semicolon-separated list of assignments for variables that are used later, for example, `init = "a=2;b=4"`. This string is evaluated only once.

`function`

Specifies an expression that is evaluated for every query. The variable that replaces the primary or lateral distance must be called `x`, for example:

```
function = "sin(x)"
function = "exp(4*x)*sin(x)"
```

In general, 1D, 2D, and 3D simple analytic functions can be specified here. The variables `x`, `y`, and `z` can be used to refer to the respective x-, y-, and z-spatial coordinates.

`value`

Specifies the default return value if the evaluation fails. The default is `1.0e18` for the primary direction and `1` when used as `LateralFunction`.

Note that:

- All defined variables are global variables. This means that, if `init="a=1"` is defined in one function, the same value will be used in all functions. Resetting the variable value in another function command will have no effect.
- You can freely mix `Eval` with `Gauss`, `Erf`, and `subMesh1D` functions.
- The symbols `"pi"` and `"e"` can be used in the expressions.
- The functions that can be used are:

```
"sin", "cos", "tan", "asin", "acos", "atan", "sinh", "cosh", "tanh", "exp",
"log", "log10", "sqrt", "floor", "ceil", "abs", "hypot", "deg", "rad"
```

- Numeric exponential constants can be specified as either `"2*10^18"` or `"2e18"`.
- As an extension to the `Eval` function, the `General` function assesses device coordinates directly, (x, y) and (x, y, z), and does not use primary and lateral distances. Any lateral functions and reference geometries (in the `Placements` section) are ignored.

Defining Submeshes

External simulation results given on a mesh can be used to define profiles in the device. The external mesh must have the same spatial dimension as the device. The datasets defined on the external mesh are interpolated to the newly generated mesh. The external profiles are called *submeshes*.

The syntax to define a submesh is:

```
SubMesh "reference name" {
   Geofile = "string"
   ...
   Fields = "string", "string", ...
}
```

where:

`Geofile`

Specifies the name of a file with an external mesh. The file must be in TDR format. The dimension of the external mesh must be the same as the dimension of the device.

NOTE Sentaurus Mesh uses a simplified version of the submesh syntax where only the `Geofile` parameter must be specified.

`Fields`

Specifies a list of fields to be extracted from the submesh. The other fields are ignored and are not used in the calculations or written to the output file.

Defining Particle Profiles

Particle definitions can be used to define profiles associated with discrete dopant distributions obtained from kinetic Monte Carlo (KMC) simulations using Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC). A continuous profile is obtained from the discrete dopant distribution by associating a doping function with each discrete dopant (see Appendix B on page 123).

The syntax to define a particle profile is:

```
Particle "reference name" {
   AutoScreeningFactor
   BoundaryExtension = value
   Divisions = value
   DopingAssignment = "CIC" | "NGP" | "Sano"
```

```
    Normalization
    NumberOfThreads = integer
    ParticleFile = "string"
    ScreeningFactor = value
    ScreeningScalingFactor = value
    Species = "string"
  }
```

where (default values are given in parentheses if applicable):

`AutoScreeningFactor`

If this option is specified, Sentaurus Mesh calculates automatically a screening factor for each discrete dopant based on the local density of dopants using $k_c = 2N(x_0, y_0, z_0)^{1/3}$, where $N(x_0, y_0, z_0)$ is the density at the location of the discrete dopant.

Even when this option is specified, `ScreeningFactor` also must be specified because, when calculating the local density, the integration box size (in micrometers) is determined using $(4.4934/\texttt{ScreeningFactor}) \times 10^4$.

`BoundaryExtension`

This parameter applies to 2D structures only and is used to obtain continuous doping on a 2D structure from a 3D KMC TDR file containing particle information.

The value given in micrometers is a thickness that is used internally to create an imaginary 3D structure by extruding the input 2D structure. This 3D structure is used to compute doping information, and this information is transferred to the 2D mesh.

`Divisions (10)`

This parameter applies to 2D structures only and is used in conjunction with the `BoundaryExtension` parameter. For each mesh point in a 2D structure, a number of points equal to a number of divisions, each separated by an equal amount, is created in the z-direction. The amount of separation is obtained by dividing the boundary extension with the number of divisions. The doping is computed on all of these points, and an average doping is assigned for the corresponding 2D mesh point.

`DopingAssignment ("Sano")`

The basic refinement method is the Sano method, but this parameter allows you to choose a method by which doping is assigned to a mesh immediately before saving the mesh:

- The cloud-in-cell (`"CIC"`) method distributes the doping of a particle to the vertex nodes of the element in which the particle is located.
- The nearest grid point (`"NGP"`) method assigns the doping of a particle to the nearest mesh node.

- The `"Sano"` method uses a doping function described in Appendix B on page 123 to distribute the doping of a particle to surrounding nodes.

`Normalization`

Specifying this option compensates for doping loss of dopants located near the boundary.

`NumberOfThreads (1)`

Parallelizes the local screening factor computation. Multithreading is recommended if the simulation contains thousands of particles.

`ParticleFile`

Specifies the name of the KMC TDR file that contains the particle (discrete dopant) information.

`ScreeningFactor`

This is the cut-off parameter, k_c, for the doping function associated with each discrete dopant (see Appendix B on page 123). The `ScreeningFactor` (given in units of cm^{-1}) can be used as a fitting parameter; however, a value for it can be estimated from $k_c = 2N^{1/3}$, where N is the impurity concentration.

`ScreeningScalingFactor`

Controls the degree of smoothness of the profile. It is applied to the screening factor when `AutoScreeningFactor` is specified.

`Species`

Specifies the name of an active impurity concentration to associate with this definition, for example, `ArsenicActiveConcentration` and `BoronActiveConcentration`.

If `Species` is not specified, all active impurities that are found in the KMC particle file will be associated with this definition.

Placements Section

The `Placements` section is composed of sets of refinement and profile instances. Their positions in the device must be specified, and they must reference a definition given in the `Definitions` section. In other words, each instance or subsection consists of the instance name, an opening brace, the specification of parameters, and a closing brace.

The order of the refinement regions in this section is important. The mesh generators select which refinement condition will be applied depending on the order of the refinement regions described in the `Placements` section.

The syntax of this section is:

```
Placements {
   Refinement "instance name" {parameters}
   Multibox "instance name" {parameters}
   Constant "instance name" {parameters}
   AnalyticalProfile "instance name" {parameters}
   SubMesh "instance name" {parameters}
   Particle "instance name" {parameters}
   ...
}
```

NOTE The order of the profile instances in the `Placements` section is important only when the `Replace` option is used.

Geometric Elements

To specify `Placements` sections, you must use geometric elements. These elements are geometric objects used to select or locate data, and they are not part of the grid elements. The coordinates of these objects are defined relative to the coordinates of the device.

The allowed geometric elements and the number of coordinate values that must be specified depend on the dimension n of the device.

Let $\vec{x} = [x_1, \ldots, x_d]$ denote a point. The following geometric elements are defined:

Point $(\vec{x}_1)$

Line $(\vec{x}_1, \vec{x}_2)$

Rectangle $(\vec{x}_1, \vec{x}_2)$

Polygon $(\vec{x}_1, \ldots, \vec{x}_m)$, $m > 2$

Complex polygon $(lump_1(polygon_1(\vec{x}_1, ..., \vec{x}_m), ..., polygon_p(\vec{x}_1, ..., \vec{x}_m))$
$lump_1(polygon_1(x_1, ..., x_m), ..., polygon_p(x_1, ..., x_m))\ )$, $m > 2$

Cuboid $(\vec{x}_1, \vec{x}_2)$

Polyhedron $\{polygon_1(\vec{x}_1, \ldots, \vec{x}_m), \ldots, polygon_p(\vec{x}_1, \ldots, \vec{x}_m)\}$, $m > 2$

Simple polygons are closed internally by adding the line segment between $\vec{x}_1 = [x_1, \ldots, x_d]$ and $\vec{x}_m = [x_1, \ldots, x_d]$. Only simple closed polyhedra are allowed. All their faces must be described.

Complex polygons are composed of lumps. Each lump represents a separate subpolygon, possibly containing holes. The first polygon inside a lump is the outer contour of the lump, while the subsequent polygons represent holes inside the lump.

The following is an example of the use of the `complexPolygon` element. The example represents two separate loops, the first of which has a hole inside:

```
AnalyticalProfile "buried n-channel" {
   Reference = "buried n-channel"
   ReferenceElement {
      Element = complexPolygon [
         lump [polygon [( 1.0 0.0 2.0 ) ( 2.0 0.0 2.0 ) ( 2.0 1.0 2.0 )
                        ( 1.0 1.0 2.0 )]
               polygon [( 1.3 0.3 2.0 ) ( 1.6 0.3 2.0 ) ( 1.6 0.6 2.0 )
                        ( 1.3 0.6 2.0 )]
         ]
         lump [polygon [( 0.0 1.5 2.0 ) ( 0.5 1.5 2.0 ) ( 0.5 2.0 2.0 )
                        ( 0.0 2.0 2.0 )]
         ]
      ]
      Direction = negative
   }
}
```

NOTE All polygons defined inside a `complexPolygon` element must be coplanar.

NOTE To describe a polyhedron with arbitrarily oriented faces, use polygons instead of rectangles.

Table 2 lists the geometric elements that can be used to specify different kinds of window in each dimension.

Table 2 Geometric elements for specifying windows

Function	1D	2D	3D
`EvaluateWindow` in `Placements` section for profiles	Line	Rectangle, Polygon	Cuboid, Polyhedron
`ReferenceElement` in `Placements` section for analytic profiles	Point	Line	Rectangle, Polygon
`RefineWindow` in `Placements` section for refinements	Line	Rectangle, Polygon	Cuboid, Polyhedron

In addition to the above-defined geometric elements, Table 3 lists other non-geometric elements that can be used to specify windows in the command file.

Table 3 Non-geometric elements for specifying windows

Element	Syntax
Material element	`material [<list of DATEX material names>]`
Region element	`region [<list of region names>]`
Composite element	`element {<list of geometric elements>}`
Sweep element	`sweepElement {<sweep element parameters>}`

Refinement or evaluation windows can be restricted to work on a particular material or region using the keyword `material` or `region`. For `material`, the argument is a valid DATEX material name in brackets. For `region`, the argument is a valid (existing) region name in brackets (see Regionwise and Materialwise Refinement on page 73).

In addition, elements can be combined to build more complex elements called *composite elements*, which are useful when defining complex reference elements for analytic profiles (see Using Composite Elements on page 72).

Sweep elements can be used to create 3D profiles by sweeping 2D profiles in 3D space. There are two types of sweep element: path sweep and angle sweep (see Creating 3D Profiles From 2D Cross Sections on page 75).

Placing Refinement Regions

In the `Placements` section, a refinement instance is specified by a name, an opening brace, the specification of parameters, and a closing brace. Several refinement instances can refer to the same set of refinement parameters.

The syntax for a refinement instance is:

```
Refinement "instance name" {
   Reference = "string"
   RefineWindow = geometric element | material [<list>] | region [<list>]
}
```

where:

`Reference`

Specifies the reference to a previously defined refinement.

`RefineWindow`

Defines the location of the refinement instance in the device. (Instead of `RefineWindow`, you can use its abbreviation `RefineWin`.) By default, `RefineWindow` is the bounding box of the device. Table 2 on page 21 lists the geometric elements that can be used. In addition, you can specify regionwise or materialwise refinement, or both refinements (see Regionwise and Materialwise Refinement on page 73).

You can specify `RefineWindow` multiple times in a `Refinement` section. When more than one `RefineWindow` is present, Sentaurus Mesh only refines the common sections of the refinement windows. This can be used to restrict the refinement to the part of a refinement box lying inside a region or material. For example:

```
Refinement "Refinement along current flow under the oxide" {
   Reference = "Refinement along current flow only in Silicon"
   RefineWin = cuboid [ ( 4.4 0 1 ) , ( 7.6 1.8 3.5 ) ]
   RefineWin = material ["Silicon"]
}
```

NOTE If no `RefineWindow` is specified, the refinement instance is used as the default region for the entire device.

Placing Multibox Regions

In the `Placements` section, a multibox instance is specified by the keyword `Multibox`, followed by the name of the multibox window and an opening brace. After the specification of parameters, a closing brace is placed. Several multibox instances can refer to the same set of multibox parameters.

The syntax for a multibox instance is:

```
Multibox "instance name" {
   Reference = "string"
   RefineWindow = geometric element
}
```

where:

`Reference`

Specifies the reference to a previously defined multibox.

`RefineWindow`

Defines the location of the refinement instance in the device. Table 2 on page 21 lists the geometric elements that can be used. By default, `RefineWindow` is the bounding box of the device.

NOTE If `RefineWindow` is not specified, the refinement instance is used as the default region for the entire device.

Placing Constant Profiles

The syntax for constant profiles is:

```
Constant "instance name" {
   Reference = "string"
   EvaluateWindow {
      Element = geometric element | material [<list>] | region [<list>]
      DecayLength = value | GaussDecayLength = value
   }
   LocalReplace
   Replace
}
```

where:

`Reference`

Specifies the reference constant to use. Only references to constant profiles are allowed.

`EvaluateWindow`

Defines the domain where the profile is evaluated and a decay length is applied in the vicinity of the window boundaries. The domain can be specified using a geometric element (see Table 2 on page 21), as well as by referring to materials or regions. (Instead of `EvaluateWindow`, you can use its abbreviation `EvalWin`.)

The decay function reduces round-off errors. It can be either an error function or a Gaussian function. To use an error function, specify `DecayLength` (or you can use its abbreviation `DecayLen`). For a Gaussian decay function, specify `GaussDecayLength`.

If `EvaluateWindow` is not defined, the transition between profiles is abrupt. If `DecayLength=0`, no decay function is applied and the transition between `EvaluateWindow` and its vicinity is abrupt. If `DecayLength` is negative, the profile is not applied to points on the border of `Element`. By default, `DecayLength=0` for all the profiles.

For analytic, constant, and particle profiles, the default value of `Element` is the bounding box of the device. For submeshes, the default value of `Element` is the bounding box of the submesh. See the equations in Appendix A on page 111 for details.

NOTE Avoid using `EvaluateWindow` when the profile is valid in the entire device and no decay function is required. The evaluation of a geometric element is time consuming.

NOTE The `DecayLength` and `GaussDecayLength` parameters do not apply to particle profiles.

`LocalReplace`

With the `Replace` option, all the computed species are set to zero and are set with the value corresponding to the given profile instance. With the `LocalReplace` option, only species defined in the corresponding `Definitions` section are set exclusively to zero and are recomputed using the current profile instance. The other species are not updated. Accordingly, the net doping contribution is updated. By default, `LocalReplace` is switched off.

`Replace`

In general, the values for each profile at each point of the newly generated mesh are computed as the sum of all profile instances defined in the `Placements` section. The instances are inspected in the same order as they are defined in the command file. If `Replace` is specified for a given instance, all current summed values are replaced by the value corresponding to the given profile instance. By default, `Replace` is switched off.

Placing Analytic Profiles

The syntax for an analytic profile is:

```
AnalyticalProfile "instance name" {
   Reference = "string"
   ReferenceElement {
      Element = element
      Direction = positive | negative
   }
   EvaluateWindow {
      Element = geometric element | material [<list>] | region [<list>]
      DecayLength = value | GaussDecayLength = value
   }
   LocalReplace
   NotEvalLine
   Replace
}
```

where:

`Reference`

Specifies the analytic profile to use. Only references to analytic profiles are allowed.

`ReferenceElement`

The direction of the normal to the `ReferenceElement` defines the direction of the analytic profile (instead of `ReferenceElement`, you can use its abbreviation `RefElem`). When evaluating the function values, the mesh points of the newly generated mesh are projected to the `Element`. The distance in the normal direction is used to evaluate the `Function`. The distance of the projection to the boundary of `Element` is used to compute the `LateralFunction`. By default, values are computed on both sides of the `Element`. If `Direction` is specified, function values are computed only on the positive or negative side of the `Element`.

In 1D devices, `Element` is a point, and the `positive` and `negative` directions are given by the coordinate axis. In 2D devices, `Element` is a line and the positive direction is taken to the right of the line.

In 3D devices, `Element` can be either a rectangle or polygon. The normal for a rectangle must be one of the coordinate axes. The `positive` and `negative` directions are defined from this axis. A (planar) polygon can be arbitrarily oriented in three dimensions. The direction is defined by the order of the points defining the polygon. A polygon is considered correctly oriented if the side of the polygon, which is surrounded by points in a positive orientation, defines the positive direction. There is no default value for `Element` and `Direction`.

`EvaluateWindow`

Restricts the placement of the analytic profile to a particular window, material, or region. See description in Placing Constant Profiles on page 24.

`LocalReplace`

See description in Placing Constant Profiles on page 24.

`NotEvalLine`

If this option is specified, the profile is not evaluated at the location of the reference element. This can be useful for placing two identical analytic profiles back-to-back using opposite directions, but without evaluating the reference element twice.

`Replace`

See description in Placing Constant Profiles on page 24.

Placing Submeshes

The syntax for references to submeshes in the `Placements` section is:

```
SubMesh "instance name" {
   Reference = "string"
   Reflect = X | Y | Z
   Rotation {
      Angle = value
      Axis = value
   }
   ShiftVector = vector
   EvaluateWindow {
      Element = geometric element | material [<list>] | region [<list>]
      DecayLength = value | GaussDecayLength = value
   }
   Ignoremat
   LocalReplace
   MatchMaterialType
   Replace
}
```

where:

`Reference`

Specifies the reference submesh to use. Only references to profiles that are defined as `SubMesh` are allowed.

`Reflect`

Specifies a reflection perpendicular to the specified coordinate axis. The allowed axes depend on the dimension of the device. The reflection point (or line or plane) is placed at the specified coordinate axis.

`Rotation`

Performs a counterclockwise rotation around the axis. The center of the rotation is the origin of the coordinate system. By default, `Angle=0`. By default, `Axis=Z` (for two and three dimensions). In one dimension, `Rotation` is not supported.

NOTE The `ShiftVector`, `Reflect`, and `Rotation` operations are performed in the order they appear in the command file. The final location and orientation of the submesh depends on this order.

`ShiftVector`

Translates a submesh to a new location. The vector is specified as two or three coordinates enclosed by parentheses.

`EvaluateWindow`

Restricts the placement of the submesh to a particular window, material, or region. See description in Placing Constant Profiles on page 24.

`Ignoremat`

If this option is specified, the material in submeshes is ignored. The standard behavior of submesh interpolation is that the interpolated value is only accepted if the point is in a region with the same material.

The option `Ignoremat` allows Sentaurus Mesh to always accept the interpolation. (By default, if the materials do not match, the closest region with the correct material is searched.) The default behavior is not checked. For example:

```
Placements {
   SubMesh "NoName_0" {
      Reference = "NoName_0"
      Ignoremat
   }
}
```

`LocalReplace`

See description in Placing Constant Profiles on page 24.

`MatchMaterialType`

When this option is specified, the submesh attempts to match equivalent material types (for example, semiconductor, insulator, conductor) instead of trying to match material names when looking up values from which to interpolate.

`Replace`

See description in Placing Constant Profiles on page 24.

Placing Particle Profiles

The syntax for placing particle profiles in the `Placements` section is:

```
Particle "instance name" {
   Reference = "string"
   EvaluateWindow {
      Element = material [<list>] | region [<list>]
```

```
    }
    LocalReplace
    Replace
  }
```

where:

`Reference`

Specifies the reference particle to use. Only references to particle profiles are allowed.

`EvaluateWindow`

See description in Placing Constant Profiles on page 24.

`LocalReplace`

See description in Placing Constant Profiles on page 24.

`Replace`

See description in Placing Constant Profiles on page 24.

Interpolate Section

The optional `Interpolate` section controls data interpolation that is performed after the mesh generators have finished.

The syntax of this section is:

```
Interpolate {
   interpolateElements = true | false
   keepTotalConcentration = true | false
   lateralDiffusion = true | false
}
```

where (default values are given in parentheses if applicable):

`interpolateElements (false)`

Interpolates element-type (scalar and vector) datasets. The element-type datasets of the input submesh are interpolated on the generated grid. The default value ignores element-type datasets.

`keepTotalConcentration (false)`

Saves the `TotalConcentration` field in the output file. By default, Sentaurus Mesh does not save this field in the output file. Sentaurus Device can calculate this field, if necessary, based on the available dopants.

`lateralDiffusion (false)`

Enables lateral extension on analytic profiles like that performed by the Synopsys Taurus™ Medici tool. This parameter affects only profiles with rectangular reference elements and attenuates the lateral decay factor by taking into account the distance from the interpolated points to all sides of the rectangle (see Lateral Error Function on page 120).

AxisAligned Section

The `AxisAligned` section controls the axis-aligned mesh generator in Sentaurus Mesh.

The axis-aligned mesh generator takes a boundary representation of the device and a series of user-defined refinement criteria, and follows these steps to create a mesh:

1. It attempts to repair the boundary using a combination of decimation and reconstruction algorithms. The algorithms are controlled by the `geometricAccuracy` parameter as well as parameters related to the Delaunay refinement for piecewise smooth complex (DelPSC) algorithm.
2. It produces an initial coarse discretization of the bounding box of the structure by applying the `xCuts`, `yCuts`, and `zCuts` parameters. This creates an initial tensor-like structure that is used as the basis for the user-defined refinement.
3. The basic mesh is refined using user-defined criteria described in Chapter 3 on page 69. Each box is bisected recursively until all resulting boxes meet the criteria specified by the user. During this process, the mesh generator ensures that criteria such as `maxAngle`, `maxAspectRatio`, and `maxNeighborRatio` are satisfied.
4. After the boxes have been refined, they are imprinted on the boundary, producing a surface axis-aligned pattern. At this stage, short surface edges and poor angles are eliminated using a combination of boundary decimation and boundary repair algorithms.
5. As the last step before delaunization, the boxes are merged with the boundary, ensuring that intersecting the boxes with the boundary does not produce an unbalanced mesh (that is, a short edge next to a long one). To control this, the algorithm uses the parameter `maxBoundaryCutRatio`.

The syntax of the `AxisAligned` section is:

```
AxisAligned {
   allowRegionMismatch = true | false
   binaryTreeSplitBox = (floatlist)
   binaryTreeSplitFactorX = integer
   binaryTreeSplitFactorY = integer
   binaryTreeSplitFactorZ = integer
   convexTriangulation = true | false
   decimate = true | false
   DelPSC = true | false
   DelPSCAccuracy = float
   DelPSCRidgeAngle = float
   DelPSCRidgeSampling = float
   fitInterfaces = true | false
   geometricAccuracy = float
   hintBoxSize = float
   imprintAccuracy = float
   imprintCoplanarFacesOnly = true | false
   imprintCoplanarityAngle = float
   imprintCoplanarityDistance = float
   latticeCellSize = (float float float)
   latticeDimensions = (integer integer integer)
   maxAngle = float
   maxAspectRatio = float
   maxBoundaryCutRatio = float
   maxNeighborRatio = float
   minEdgeLength = float
   minimumRegionMismatchVolume = float
   overscan = true | false
   overscanResolution = float
   skipSameMaterialInterfaces = true | false
   smoothing = true | false
   spacingMethod = even | regular | smooth
   splitDisconnectedRegions = true | false
   virtualSpacing = true | false
   xCuts = (floatlist)
   yCuts = (floatlist)
   zCuts = (floatlist)
}
```

where (default values are given in parentheses if applicable):

`allowRegionMismatch (false)`

If `allowRegionMismatch = true`, when Sentaurus Mesh checks whether the number of regions in the input boundary and the number of regions at the end of the meshing process are the same, if there is a difference between the numbers of regions, Sentaurus Mesh will ignore the discrepancy, and the meshing process will continue.

If `allowRegionMismatch = true` and `minimumRegionMismatchVolume` has also been specified, Sentaurus Mesh checks the volumes of all deleted regions:

- If the volume of a deleted region is *less than the value* specified by `minimumRegionMismatchVolume`, the meshing process will continue and the number of deleted regions is reported.
- If the volume of a deleted region is *greater than the value* specified by `minimumRegionMismatchVolume`, the meshing process will stop.

If `allowRegionMismatch = false`, when Sentaurus Mesh checks whether the number of regions in the input boundary and the number of regions at the end of the meshing process are the same, if there is a difference between the numbers of regions, the meshing process will stop.

`binaryTreeSplitBox`

Specifies a box that defines the region where `binaryTreeSplitFactorX`, `binaryTreeSplitFactorY`, and `binaryTreeSplitFactorZ` are applied. By default, no box is used.

For 2D simulations, `binaryTreeSplitBox` is set to:

```
(xmin <float> ymin <float> xmax <float> ymax <float>)
```

For 3D simulations, `binaryTreeSplitBox` is set to:

```
(xmin <float> ymin <float> zmin <float> xmax <float> ymax <float> zmax <float>)
```

`binaryTreeSplitFactorX (1)`

Instructs Sentaurus Mesh to split the final binary tree used in the refinement step by a specified factor in the x-direction. This factor must be a power of 2; otherwise, the nearest power of 2 will be used. This parameter can be used to achieve an approximately uniform mesh refinement in the x-direction.

`binaryTreeSplitFactorY (1)`

Same as `binaryTreeSplitFactorX` but in the y-direction.

`binaryTreeSplitFactorZ (1)`

Same as `binaryTreeSplitFactorX` but in the z-direction.

`convexTriangulation (false)`

Creates a minimum triangulation of a 3D model containing convex regions. The input 3D boundary must be a convex model. Since the goal is to create a minimum triangulation of the convex model, the refinement specifications in the command file (if any) are ignored. If the input model contains nonconvex regions, the meshing terminates with a corresponding message.

`decimate (true)`

Specifies whether the 3D boundary is decimated. The decimation process removes nodes from the surface, thereby generating a simpler structure. A node is removed only if the deformation caused by removing the node is less than the value specified by the `geometricAccuracy` parameter.

`DelPSC (false)`

Instructs Sentaurus Mesh to apply the DelPSC algorithm to boundary surfaces. It is useful for curved surfaces. If `IOControls{numThreads=integer}` is specified, the DelPSC algorithm uses multithreading. See [1][2] for a description of the algorithm.

`DelPSCAccuracy (0.0001)`

Controls the deviation (given in µm) between the new curved surface and the original curved surface in the DelPSC algorithm. The new curved surface can deviate from the original curved surface by, at most, the value of `DelPSCAccuracy`. New vertices lie exactly on the original surface, but new triangles cannot lie exactly on the original surface *unless* the original surface is flat. In general, the smaller the value of `DelPSCAccuracy` is, the smoother the new surface becomes, and the more accurate the new surface represents the original surface.

In general, setting `DelPSCAccuracy` to 2% of the radius of curvature is appropriate. Larger values allow the DelPSC algorithm to run faster but generate coarser discretization on curved surfaces. Smaller values make the DelPSC algorithm run slower and generate finer discretization on curved surfaces.

`DelPSCRidgeAngle (150)`

Angle used by the DelPSC algorithm to determine geometric features.

`DelPSCRidgeSampling (0.01)`

Controls the size (given in µm) of small triangles on curved surfaces in the DelPSC algorithm.

In general, setting `DelPSCRidgeSampling` to 10% of the radius of curvature is appropriate. Larger values allow the DelPSC algorithm to run faster but generate bigger triangles next to geometric features and triple lines on curved surfaces. Smaller values make the DelPSC algorithm run slower and generate smaller triangles next to geometric features and triple lines on curved surfaces.

`fitInterfaces (false)`

Instructs Sentaurus Mesh to calculate the `xCuts`, `yCuts`, and `zCuts` automatically by first refining along the axis-aligned interfaces.

`geometricAccuracy (1e-6)`

Restricts the changes to the boundary, which are undertaken by the decimation algorithm. The decimation algorithm is not allowed to modify the boundary more than the value of `geometricAccuracy` given in µm.

`hintBoxSize (1.0)`

When overscanning analytic profiles, Sentaurus Mesh calculates a *hint box* containing the peak value. The size of this box is a number of standard deviations from the peak. The default is one standard deviation around the peak value.

`imprintAccuracy (1e-5)`

Distance used to determine whether two points are too close during axis-aligned imprinting.

`imprintCoplanarFacesOnly (true)`

If this option is switched on, Sentaurus Mesh imprints the axis-aligned refinement only on faces that are away from curved regions of the boundary. This is useful to avoid overrefinement in curved areas.

`imprintCoplanarityAngle (179.9)`

Angle used by the face-imprinting algorithm to determine whether two boundary faces are coplanar.

`imprintCoplanarityDistance (1e-5)`

Distance used by the face-imprinting algorithm to determine whether two faces are coplanar.

`latticeCellSize`

Specifies a tensor-like tessellation of the structure with a spacing that is as close as possible to the defined cell size. If the `virtualSpacing` parameter is used, the generated lines guide the refinement algorithm, but not all of these lines will necessarily be present in the final mesh.

`latticeDimensions`

Specifies a tensor-like tessellation of the structure with the defined number of lines along each direction. If the `virtualSpacing` parameter is used, the generated lines guide the refinement algorithm, but not all of these lines will necessarily be present in the final mesh.

`maxAngle (90` in 2D, `165` in 3D`)`

Determines the maximum angle produced in the binary tree. In two dimensions, the default is 90°.

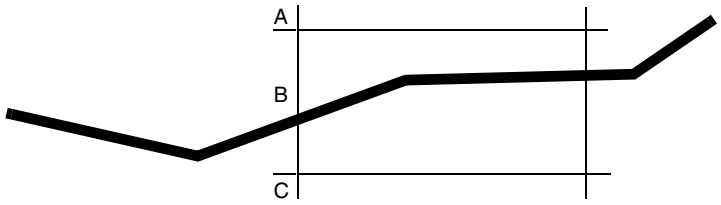
`maxAspectRatio (1e6)`

Specifies the maximum aspect ratio allowed in the elements of the binary tree at the end of the refinement step.

`maxBoundaryCutRatio (0.01)`

Defines the maximum-allowed ratio between adjacent segments on an axis-aligned box intersecting the boundary. When a segment belonging to an axis-aligned box intersects the boundary and the resulting cuts have a higher ratio than specified by this parameter, all axis-aligned faces associated with this segment are disabled and are not allowed in the final mesh.

For example, in the following figure, a candidate axis-aligned segment AC can intersect a boundary edge at point B such that the AC segment becomes two colinear segments AB and BC.



In the absence of `maxBoundaryCutRatio` (value `0`), the ratio of the lengths of these edges would be unconstrained. With this parameter, the ratio between the short segment and the long segment are determined: either AB/AC or BC/AC. If either of these lengths is less than `maxBoundaryCutRatio`, the AC segment and any other segment connected to it are rejected and do not appear in the final mesh. In the case of a 3D mesh, this means that any axis-aligned face touching this segment is disabled and cannot appear in the final mesh.

Setting `maxBoundaryCutRatio` to a high value (closer to 1) reduces the possibility of having sharp changes in mesh sizes across the boundary. However, at the same time, it may create holes in the mesh since, potentially, many axis-aligned faces or segments may be disabled. Setting `maxBoundaryCutRatio` to a small value reduces the possibility of holes around the boundary of the device, but it will produce sharp transitions in the mesh size at the boundary.

`maxNeighborRatio (2` in 2D, `4` in 3D`)`

Specifies the size ratio between adjacent elements.

`minEdgeLength (1e-7)`

Specifies the minimum edge length (given in μm) produced on the boundary before the delaunization step.

`minimumRegionMismatchVolume (0)`

Specifies a region volume that Sentaurus Mesh uses when checking deleted regions. It is used in conjunction with `allowRegionMismatch=true`.

`overscan (false)`

Instructs Sentaurus Mesh to scan the axis-aligned cells for field changes that justify more refinement based on the user parameters. The algorithm creates a small tensor mesh with the resolution indicated by the `overscanResolution` parameter and uses it to check for fine variations in the field profiles.

To avoid scanning all cells, the tool obtains 'hints' from the profiles as to where the interesting areas are located. For this purpose, the tool internally calculates the location of the peak values and p-n junctions, and gives them as a hint to the mesh generator.

`overscanResolution (0.3)`

Resolution used to scan the device for field changes. The algorithm takes each unrefined cell and virtually subdivides it into smaller cells. Then, these small cells are checked for changes in the field values that justify more refinement.

`skipSameMaterialInterfaces (false)`

During refinement, if this parameter is set to `true`, Sentaurus Mesh ignores interfaces that have the same material on both sides.

`smoothing (true)`

Specifies whether the binary tree will be graded using the `maxAspectRatio` and `maxNeighborRatio` parameters.

`spacingMethod (even)`

Specifies the type of progression used by the refinement algorithm when expanding the refinement specified between lines:

- `even`: Distributes the cuts evenly, trying to approximate the spacing specified at the beginning of the interval.
- `regular`: Distributes the cuts evenly using the exact spacing specified at the beginning of the interval, and leaving the last interval with an approximate size if there is no more room to accommodate the requested size.
- `smooth`: Distributes the cuts to have a smooth grading of spacing between lines.

`splitDisconnectedRegions (false)`

If an input boundary contains regions with multiple disconnected parts, this parameter specifies whether these regions should be split into multiple disconnected regions and renamed according to Sentaurus Process naming rules, or whether these regions and their names should be preserved.

`virtualSpacing (false)`

Specifies whether the expansion lines produced by pairs of values defined by the `xCuts`, `yCuts`, and `zCuts` parameters will be either explicit lines or virtual lines that guide the refinement algorithm. When the lines are virtual, the refinement algorithm snaps the refinement coordinates to these lines instead of using the standard bisection algorithm. This allows the refinement to conform to a more user-defined pattern.

`xCuts, yCuts, zCuts`

These values represent refinement lines that are introduced into the mesh before any user-defined refinement. The lines define a rectilinear grid from which to start the refinement. Since each box in the initial grid is refined independently, different regions of the device can be isolated, thereby obtaining a more predictable refinement in each one of them. The cuts in each direction are specified as a list of cut points enclosed in parentheses.

Each cut point can be either a single floating-point value or a pair of floating-point values. A single value indicates the position of the cut point. When a pair of values is used, the first value indicates the position of the cut point, and the second value indicates the expansion of the cuts into a sequence of lines to be generated between adjacent pairs of lines.

The following example creates a series of grid lines located at 0, 1, and 2 µm. Between 0 and 1 µm, the series of lines should have a spacing of 0.1 (10 lines). Between 1 and 2 µm, the series of lines should have a spacing of 0.2 (5 lines):

```
xCuts = ( (0 0.1) (1 0.2) 2)
spacingMethod = even
```

The `spacingMethod` and `virtualSpacing` parameters control the refinement algorithm.

By default, no cuts are introduced into the mesh unless the `xCuts`, `yCuts`, or `zCuts` parameter is used.

Offsetting Section

The offsetting mesh generator uses the `Offsetting` section to create meshes with layers that follow the device interfaces. The layers are combined with the axis-aligned mesh generated by the axis-aligned mesh generator (see AxisAligned Section on page 30). The offsetting mesh

generator first produces an axis-aligned mesh and then adds the offsetting layers on top of that mesh, clearing the axis-aligned elements that overlap the layers.

NOTE Specify either the `EnableOffset` or `EnableSections` option in the `IOControls` section of the command file to enable the offsetting mesh generator (see IOControls Section on page 6).

The syntax of the `Offsetting` section is:

```
Offsetting {

   # offsetting-global-section:
   noffset {
      factor = float
      hlocal = float
      maxlevel = integer
   }

   # offsetting-interface-section:
   noffset material | region "string" "string" {
      factor = float
      hlocal = float
      window = [(float float float) (float float float)]
   }
   # offsetting-region-section:
   noffset material | region "string" {
      maxlevel = integer
   }
}
```

where (default values are given in parentheses if applicable):

`factor (1.3)`

As the front progresses, the thickness of the layers increases by this factor.

`hlocal (0)`

Thickness of first layer in µm. The default `hlocal=0` means no layering at all.

`maxlevel (200)`

Specifies the number of layers that offsetting creates. If the front collides with other fronts or surfaces, the mesh generator stops prematurely.

`window`

Specifies the cuboid used to confine the creation of layering. For a large interface, this parameter allows you to limit the layering to a spatial region of interest, thereby reducing

the size of the grid. Note that `window` controls only the start of the layering and, therefore, the layers may grow outside of the window. Multiple windows can be specified within the *`offsetting-interface`* section.

The parameters `hlocal` and `factor` affect the material interfaces and surfaces. They can be specified on an interface basis using the syntax with two region names. The syntax is not symmetric:

- `noffset region "A" "B" {}` applies to the layers in region `A` where it borders region `B`.
- `noffset region "B" "A" {}` sets parameters for the other side of the same interface.

At places where contacts are defined, their names are used to define interfaces. The pseudo–region name `Exterior` is used for surfaces.

The parameter `maxlevel` can be set only per region using the syntax with one region name.

NOTE In both cases, you can use region names (keyword `region`) or the material property (keyword `material`). Since the material property is more persistent, it is advisable to use it instead of region names.

NOTE It is recommended to specify refinement criteria in the `Definitions` and `Placements` sections of the command file. Otherwise, the resulting mesh will be very coarse.

NOTE It is recommended to use a small number of layers to reduce spurious refinements near the curved interfaces during delaunization of the mesh.

Delaunizer Section

The `Delaunizer` section controls the behavior of the delaunization algorithms in Sentaurus Mesh. The syntax of this section is:

```
Delaunizer {
   coplanarityAngle = float
   coplanarityDistance = float
   delaunayTolerance = float
   edgeProximity = float
   faceProximity = float
   maxAngle = float
   maxConnectivity = float
   maxNeighborRatio = float
   maxPoints = integer
   maxSolidAngle = float
   maxTetQuality = float
   minAngle = float
```

```
    minEdgeLength = float
    sliverAngle = float
    sliverDistance = float
    sliverRemovalAlgorithm = integer
    storeDelaunayWeight = true | false
    type = boxmethod | conforming | constrained
  }
```

where (default values are given in parentheses if applicable):

`coplanarityAngle (175)`

Determines whether two adjacent boundary faces are coplanar. The floating-point number represents the angle between the faces.

`coplanarityDistance (1e-5)`

Determines whether two adjacent boundary faces are coplanar. The floating-point number (given in µm) represents the absolute deformation made to the surface when the common edge is flipped.

`delaunayTolerance (1e-4)`

Specifies how close the ridges and boundary faces conform to the Delaunay criterion. A value of 0 everywhere implies a very strict Delaunay criterion. A value of 1 everywhere is equivalent to the construction of a constrained Delaunay triangulation (CDT). See Delaunay Tolerance on page 42.

`edgeProximity (0.05)`

Specifies the minimum ratio of the length of a new edge to the length of the parent edge from which it was generated. If an edge AB will be refined at point C and one of the ratios AC/AB or CB/AB is smaller than `edgeProximity`, point C is moved to the center of AB. When this value approaches 0.5, the edges will be more isotropically refined and the final mesh may contain many more points.

`faceProximity (0.05)`

Specifies the minimum ratio of the area of a new face to the area of the parent face from which it was generated. If a face ABC will be refined at point D and one of the ratios AD/r, BD/r, or CD/r is smaller than `edgeProximity` (where r is the radius of the circumscribed sphere), point D is moved to the Voronoï center of ABC. When this value approaches 0.5, the faces will be more isotropically refined and the final mesh may contain many more points.

`maxAngle (180)`

Specifies the maximum angle allowed in the elements of the mesh (2D only).

`maxConnectivity (1e+30)`

Specifies the number of edges that can be connected to a mesh point.

`maxNeighborRatio (1e+30)`

Specifies the maximum-allowed ratio between the circumscribed spheres of neighboring elements. Values close to `2` should give a better grading, but they may also increase the mesh size considerably.

`maxPoints (500000)`

Sets a limit on the maximum number of points that the delaunizer generates. The limit is observed after the ridges have been recovered.

`maxSolidAngle (360)`

Specifies the maximum solid angle allowed in the elements of the mesh (3D only).

`maxTetQuality (1e37)`

Specifies the maximum circumscribed sphere radius–to–shortest edge ratio allowed in the mesh (3D only).

`minAngle (360)`

Specifies the minimum angle allowed in the elements of the mesh (2D only).

`minEdgeLength (1e-9)`

A floating-point number (given in μm) used to display a warning when the surface edges become too short.

`sliverAngle (175)`

Controls the elimination of slivers. The sliver elimination algorithm removes all elements where the maximum dihedral angle exceeds this value (given in degrees). The algorithm endeavors to achieve this goal but, in general, it may not be possible. In practice, the final meshes contain elements where the maximum dihedral angle is approximately $179°$.

`sliverDistance (1e-2)`

Controls the amount of damage performed by the sliver elimination algorithm (see Eliminating Slivers on page 109). The value specifies the maximum weight used at a given node.

`sliverRemovalAlgorithm (1)`

Selects the sliver elimination algorithm:

- `1` selects the original algorithm.
- `2` selects the new algorithm that reduces the number of non-Delaunay elements by assigning more appropriate weights to vertices (see Eliminating Slivers on page 109).

`storeDelaunayWeight (false)`

Stores the nodal weight from the sliver elimination algorithm in the output file as a field variable when set to `true`. By supplying the Delaunay weight to Sentaurus Device, the box method library will have better convergence. This field variable is called the Delaunay–Voronoï weight (`DelVorWeight`) with the unit of μm^2 in the TDR file.

`type (boxmethod)`

Specifies the type of Delaunay mesh that the delaunization algorithm constructs:

- The `boxmethod` option imposes very strict conditions on the boundaries. The smallest circumscribed sphere around the boundary faces and ridges must be free of points.
- With the `conforming` option, the conditions at the boundary are more relaxed. This means that there exists a circumscribed sphere around a boundary face, which is free of points. This is equivalent to the standard Delaunay condition.
- When the `constrained` option is specified, the boundary faces are inserted into a Delaunay mesh of the input points using a CDT algorithm. This option produces the least refinement of all options, but it produces meshes that are not suitable for device simulation.

Delaunay Tolerance

The tolerance used to calculate the Delaunay criterion can be adjusted locally based on `region`, `material`, or `window` information:

```
boundary material | region "string" "string" {
   delaunayTolerance = float
   window = { (float, float, float) (float, float, float) }
}

surface material | region "string" {
   delaunayTolerance = float <WINDOW>
}

interior material | region "string" {
   delaunayTolerance = float <WINDOW>
}
```

The `delaunayTolerance` parameter in the `boundary`, `surface`, and `interior` subsections must always be specified. The `window` parameter is optional. These subsections do not accept any other parameters (that is, you cannot restrict the values of parameters such as `maxPoints` and `minEdgeLength` in regions or materials individually).

The following examples show the use of the Delaunay tolerance parameters:

```
Delaunizer {
   # relax the tolerance at the boundary between any two materials
   boundary {
      delaunayTolerance=1
   }

   # restrict the tolerance at the boundary between silicon and oxide
   boundary material "Oxide" "Silicon" {
      delaunayTolerance = 1e-4
   }

   # relax the tolerance in the interior of the device
   interior {
      delaunayTolerance = 1
   }

   # restrict the tolerance around the gate area
   interior region "gate" {
      delaunayTolerance = 1
      window = {(0.1,0,0) (0.2,0.1,0.1)}
   }
}
```

Tensor Section

The `Tensor` section can contain the following subsections and controls the tensor-product mesh generator:

```
Tensor {
   Mesh {parameters}
   EMW {parameters}
   Box {parameters}
}
```

NOTE To activate the `Tensor` section, specify the `EnableTensor` option in the `IOControls` section of the command file (see IOControls Section on page 6).

Mesh Subsection for Controlling Mesh Generation

Various parameters can be defined in the `Mesh` subsection of a `Tensor` section of the command file. These parameters control mesh generation. The syntax of a `Mesh` subsection is:

```
Tensor {
   Mesh {
      axisAlignedFeatureAngle = float
      doping
      grading = {float float float}
      grading off
      maxCellSize = float
      minCellSize = float
      maxBndCellSize = float
      minBndCellSize = float
      minNumberOfCells = integer
      numPoints = integer
      numPointsX = integer
      numPointsY = integer
      numPointsZ = integer
      scale = {float float float}
      window "string" float float float float float float
      xCuts = (floatlist)
      yCuts = (floatlist)
      zCuts = (floatlist)
   }
}
```

where (default values are given in parentheses if applicable):

`axisAlignedFeatureAngle (0.5 degrees)`

Part of the process of generating the refinement involves refining the grid at the location of axis-aligned interfaces found on the boundary. If there are boundary faces that are not nearly axis-aligned, the refinement algorithm ignores them, leading to unexpected holes in the refinement.

The `axisAlignedFeatureAngle` parameter allows you to specify a tolerance to indicate to the tool which faces should be considered axis aligned. The tool measures the deviation between the face normal and the nearest coordinate axis. If the deviation is smaller than `axisAlignedFeatureAngle`, the face is considered a feature and one of its points will be added to the coordinates used when refining the mesh.

`doping`

For EMW applications, doping is generally not required.

When the `EnableEMW` option is specified in the `IOControls` section of the command file, doping is switched off to avoid unnecessary doping operations that may take too much CPU time. If doping is required, the `doping` option can be used in the `Mesh` subsection to trigger doping. By default, for typical applications, doping is switched on.

`grading (1.25)`

Specifies the grading in each direction. The default is 1.25 in each direction. This can be specified in the following way:

- In three dimensions: `grading = {`*`gradx grady gradz`*`}`
- In two dimensions: `grading = {`*`gradx grady`*`}`

NOTE If the `grading` parameter is specified in both the `Mesh` subsection and the `EMW` subsection, the `EMW` subsection takes precedence.

`grading off`

This statement switches off the grading refinement. By default, grading is switched on.

`maxCellSize`

Specifies the maximum cell size allowed in a region. The default cell size in each direction is 10% of the geometry model size in that direction.

`minCellSize (1e-4)`

Specifies the minimum cell size (given in µm) allowed in a region.

`maxBndCellSize`

Specifies the maximum cell size (given in µm) perpendicular to each material interface on the boundary. For this parameter, a normal vector is computed for each material interface on the boundary, and a direction of the maximum projection is found. Cells are clustered next to the material interface in the direction of the maximum projection. The default cell size in each direction is 10% of the geometry model length in that direction.

In addition, you can restrict `maxBndCellSize` to an interface by specifying an interface option as follows:

```
maxBndCellSize interface material | region "string" "string" float
```

To address external boundaries, you can use the keyword `"Exterior"` as one of the materials or regions of an interface. For example:

```
maxBndCellSize interface material "Silicon" "Exterior" float
maxBndCellSize interface region "substrate" "Exterior" float
```

By default, if neither material `"Exterior"` nor region `"Exterior"` is specified, exterior interfaces are not affected.

`minBndCellSize (1e-4)`

Specifies the minimum cell size (given in µm) perpendicular to a material interface on the boundary. For this parameter, a normal vector is computed for each material interface on the boundary, and a direction of the maximum projection is found. The cell size next to the material interface in the direction of the maximum projection will be, at least, the value of `minBndCellSize`.

In addition, you can restrict `minBndCellSize` to an interface in the same way as for `maxBndCellSize`.

`minNumberOfCells (0)`

Specifies the minimum number of cells required in each region and in each direction. The actual number of cells is not necessarily the same as the value of `minNumberOfCells` due to other parameters such as `maxCellSize` (default 10% of the entire structure) and `minCellSize` (default `1e-4` µm). The refinement algorithm for `minNumberOfCells` is based on adaptive bisection, so cell sizes are not necessarily equidistant. If you want the cell sizes to be equidistant, use `maxCellSize`.

`numPoints`

Specifies the fixed number of points in all directions.

`numPointsX`

Specifies the fixed number of points in the x-direction.

`numPointsY`

Specifies the fixed number of points in the y-direction.

`numPointsZ`

Specifies the fixed number of points in the z-direction.

`scale (1)`

Specifies a mesh scaling factor. This parameter can be used to convert the mesh into different units and can be specified in the following way:

- In three dimensions: `scale = {`*`sx sy sz`*`}`
- In two dimensions: `scale = {`*`sx sy`*`}`

`window`

Restricts the effects of the refinement parameters. The syntax for defining a window is the following way:

- In three dimensions: `window "windowname" xmin xmax ymin ymax zmin zmax`
- In two dimensions: `window "windowname" xmin xmax ymin ymax`

`xCuts, yCuts, zCuts`

The values represent cuts in the tensor mesh where the refinement starts. These cuts are kept as part of the final tensor mesh. The cuts in each direction are specified as a list of double-precision values enclosed in parentheses. By default, no cuts are introduced into the tensor mesh.

You can specify these refinement parameters (except for `numPoints`, `numPointsX`, `numPointsY`, and `numPointsZ`) for a region, material, direction, or window, in any of the following ways:

For all regions, in all directions	`parameter = floatOrint`
In a region, in all directions	`parameter region "regionname" floatOrint`
In a material, in all directions	`parameter material "materialname" floatOrint`
In a window, in all directions	`parameter window "windowname" floatOrint`
For all regions, in a direction	`parameter direction "x | y | z" floatOrint`
In a region, in a direction	`parameter region direction "regionname" "x | y | z" floatOrint`
In a material, in a direction	`parameter material direction "materialname" "x | y | z" floatOrint`
In a window, in a direction	`parameter window direction "windowname" "x | y | z" floatOrint`

Sometimes, the same parameter is assigned a value multiple times, in which case, the last assignment is taken into consideration.

Before specifying a parameter to be applied to a window, that window must be defined inside a `Mesh` subsection of the command file. If a parameter specified through the `window` option overlaps parameters specified with other options, the smallest of these parameters is considered while meshing.

EMW Subsection for Computing Cell Size Automatically

When generating tensor meshes, the maximum cell sizes are computed automatically when the `EnableEMW` option is specified in the `IOControls` section of the command file. This application applies to Sentaurus Device Electromagnetic Wave Solver (EMW). The size computed is a function of wavelength, nodes per wavelength, and the magnitude of a complex refractive index (CRI).

The required parameters are specified in the `EMW` subsection of the `Tensor` section of the command file. The syntax of the `EMW` subsection is:

```
Tensor {
   EMW {
      parameter filename = "string"
      CRIMIPATH = "string"
      CRIMODEL = "string"
      CRI WavelengthDep Real Imag
      grading = {float float float}
      grading off
      NoEMWSolverConstraintsCheck
      wavelength = float
      wavefrequency = float
      CRI region "regionName" WavelengthDep Real Imag
      CRI material "materialName" WavelengthDep Real Imag
      CRI region "regionName" CRIMODEL "string"
      CRI material "materialName" CRIMODEL "string"
      npw | nodeperwavelength {
         material "materialName" value
         material direction "materialName" "x | y | z" float
         region "regionName" float
         region direction "regionName" "x | y | z" float
      }
      npw  | nodeperwavelength  = integer
      npwx | nodeperwavelengthX = integer
      npwy | nodeperwavelengthY = integer
      npwz | nodeperwavelengthZ = integer
   }
}
```

where (default values are given in parentheses if applicable):

`parameter filename = "string"`

This statement sets the parameter `filename` that contains the CRI table of materials that are present in the input structure.

`CRIMIPATH`

(Optional) Specifies the location of the CRI model.

`CRIMODEL`

(Optional) Specifies the name of the CRI model.

`CRI WavelengthDep Real Imag`

This statement sets the wavelength dependency on the real part, or the imaginary part, or both parts of the CRI values. The specification of real and imaginary statements is optional. Some examples are:

- Set the wavelength dependency only on the real part of the CRI:

  ```
  CRI WavelengthDep Real
  ```

- Set the wavelength dependency only on the imaginary part of the CRI:

  ```
  CRI WavelengthDep Imag
  ```

- Set the wavelength dependency on both the real and imaginary parts of the CRI:

  ```
  CRI WavelengthDep
  ```

`grading (1.25)`

Specifies the grading in each direction. The default is 1.25 in each direction. This can be specified in the following way:

- In three dimensions: `grading = {`*`gradx grady gradz`*`}`
- In two dimensions: `grading = {`*`gradx grady`*`}`

NOTE If the `grading` parameter is specified in both the `Mesh` subsection and the `EMW` subsection, the `EMW` subsection takes precedence.

`grading off`

This statement switches off the grading refinement. By default, grading is switched on.

`NoEMWSolverConstraintsCheck`

Sentaurus Device Electromagnetic Wave Solver (EMW) has two limitations in handling tensor meshes:

- It cannot handle tensor meshes with holes inside the structure.
- There must be at least one cell in each direction in a region.

By default, if these conditions are not met after generating the mesh, Sentaurus Mesh exits with an error message.

During preprocessing, the tensor-product mesh generator attempts to determine whether there will be at least one cell along a given direction inside a region before the tensor mesh is constructed. This is not always possible, especially if regions have complicated geometries.

This check is performed to save time before generating a tensor mesh, especially for large structures.

If the tensor-product mesh generator detects a problem during preprocessing, it will continue with mesh generation while issuing a warning message such as:

```
Warning: EMW applications require a minimum of 1 cell in each direction.
Region gate of material Oxide might not satisfy this condition in X direction.
Make sure that minCellSizeX for this region is at most 0.01
(or slightly smaller) to account for round-off errors.
You can do that by explicitly setting minCellSizeX, or through _numPointsX.
```

Using the `NoEMWSolverConstraintsCheck` option disables all of these checks.

`wavelength (0.555)`

Specifies the wavelength in micrometers.

`wavefrequency`

Specifies the value of the wavelength frequency. The wavelength is computed using this value and the speed of light.

`CRI region "`*`regionName`*`" WavelengthDep Real Imag`

This statement sets the wavelength dependency for a specified region. Some examples are:

- Set the wavelength dependency for this region only on the real part of the CRI:

  ```
  CRI region "Silicon_0" WavelengthDep Real
  ```

- Set the wavelength dependency for this region only on the imaginary part of the CRI:

  ```
  CRI region "Silicon_0" WavelengthDep Imag
  ```

- Set the wavelength dependency for this region on both the real and imaginary parts of the CRI:

  ```
  CRI region "Silicon_0" WavelengthDep
  ```

`CRI material "`*`materialName`*`" WavelengthDep Real Imag`

This statement sets the wavelength dependency for this material.

`CRI region "`*`regionName`*`" CRIMODEL "`*`string`*`"`

This statement sets a CRI model for a specified region.

`CRI material "materialName" CRIMODEL "string"`

This statement sets a CRI model for a specified material.

`npw | nodeperwavelength (10)`

This subsection defines the nodes per wavelength according to region or material, and in a direction. If the direction is not used, the value is used in all directions. For example, the following statement defines nodes per wavelength in silicon material in the x-direction:

```
npw { material direction "Silicon" "x" 20 }
```

The default value of the nodes per wavelength is 10 in all directions for each material.

For a given material, the cell size is computed using the formulas:

$$\lambda_{mat} = \frac{\text{wavelength}}{R_{mod}} \quad (1)$$

$$\text{cellsize}_{mat} = \frac{\lambda_{mat}}{\text{npw}} \quad (2)$$

The parameter R_{mod} Eq. 1 is computed depending on the settings of the `ComplexRefractiveIndex` model:

- If `WavelengthDep Real` is used, $R_{mod} = |n|$.
- If `WavelengthDep Imag` is used, $R_{mod} = |k|$.
- If `WavelengthDep Real Imag` is used, $R_{mod} = \sqrt{n^2 + k^2}$.

Here, n is the real part and k is the imaginary part of the CRI.

`npwx | nodeperwavelengthX`

Sets the nodes per wavelength similar to `npw` but only in the x-direction for all materials.

`npwy | nodeperwavelengthY`

Sets the nodes per wavelength similar to `npw` but only in the y-direction for all materials.

`npwz | nodeperwavelengthZ`

Sets the nodes per wavelength similar to `npw` but only in the z-direction for all materials.

Box Subsection for Plotting

New regions can be added to the tensor mesh that can be used for plotting purposes in EMW applications. The new regions are specified by the `Box` subsection of the `Tensor` section of the command file.

Any number of `Box` subsections can be specified in the `Tensor` section of the command file. The `Box` subsections are added outside the `Mesh` subsection.

The syntax of the `Box` subsection is:

```
Tensor {
   Box {
      boundingBox
      boundingBox region = "string"
      endPoint = {float float float}
      exact = "yes" | "no"
      material = "string"
      name = "string"
      startPoint = {float float float}
      tolerance = float
   }
}
```

where (default values are given in parentheses if applicable):

`boundingBox`

This option can be used instead of specifying `startPoint` and `endPoint`. It automatically sets the minimum and maximum of the structure bounding box as the `startPoint` and `endPoint`, respectively.

`boundingBox region = "string"`

This statement can be used instead of specifying `startPoint` and `endPoint`. It automatically sets the minimum and maximum of the region bounding box as the `startPoint` and `endPoint`, respectively.

`endPoint`

Specifies the highest point of the bounding box used for the plot (*`xmax ymax zmax`*).

`exact ("no")`

If `exact="yes"`, the resultant mesh should contain nodes whose coordinates match `startPoint` and `endPoint`. If `exact="no"`, the nodes that are closest to `startPoint` and `endPoint` are written in the tensor mesh.

`material ("none")`

If not specified, the name of the material defaults to `"none"`.

`name`

Name of this region.

`startPoint`

Specifies the lowest point of the bounding box used for the plot (*`xmin ymin zmin`*).

`tolerance`

The tolerance is used only if `exact="yes"`. The tolerance value indicates that the box should be aligned to any existing boundary or cell interface within this tolerance distance. This avoids unnecessary small cells locally. A value of model length in each direction multiplied by 1e-4 µm is used as the default.

In two dimensions, `tolerance= {`*`tx, ty`*`}`.

In three dimensions, `tolerance= {`*`tx, ty, tz`*`}`.

Tools Section

The `Tools` section is used to execute geometric operations on either a boundary file or a mesh file. The input mesh can be either a tetrahedral mesh or a hybrid (mixed-element) mesh.

If a hybrid mesh is used, it must be converted to a tetrahedral mesh before applying the tool (see Converting a Tetrahedral Mesh to a Hybrid Mesh on page 60). The mesh is converted back to a hybrid mesh after all operations have been executed. If an operation such as a simple transformation is applied, the resulting mesh might differ slightly from the original mesh, despite no topological changes.

The operations are executed according to their order in the `Tools` section. The output of one operation becomes the input for the next operation.

The syntax of the `Tools` section is:

```
Tools {
   parameters
}
```

NOTE To use the `Tools` section, you must specify the `EnableTools` option in the `IOControls` section of the command file (see IOControls Section on page 6).

Appending the Input Structure

This section appends the input structure periodically at the specified position:

```
Tools {
   Append {
      axis = xmin | ymin | zmin | xmax | ymax | zmax
      map "stringA" = "stringB"
   }
}
```

NOTE It works only for 2D and 3D boundaries.

Creating Profiles

This section creates profiles in the input mesh with the description given in the command file:

```
Tools {
   CreateProfiles {
      SrcMesh = "string"
      CmdFile = "string"
   }
}
```

The mesh is not modified in this process as the refinement specifications in the command file are ignored. During profile creation, the existing profiles in the input mesh, which are again specified in the command file, will only be recreated. The rest of the profiles are untouched.

Setting a Transformation

This section sets a transformation matrix to a mesh or a boundary:

```
Tools {
   Set Transformation {
      translation = (float float [float])
      scale = float | scale = (float float float)

      rotation {
         axis = (float float float)
         angle = float
      } |
      rotation {
         matrix (float float float float float float float float float)
      }
```

```
   }

   Apply Transformation
}
```

NOTE The `Set Transformation` operation applies to both the mesh and boundary.

A translation vector is used to set a translation. The rotation can be set by either an axis vector and an angle in degrees, or a matrix. A mesh or a boundary also can be scaled by specifying a floating-point value or a vector.

The `Apply Transformation` statement applies the transformation that is set.

Removing Short Features

This section removes unwanted short features in a boundary:

```
Tools {
   Decimate {
      accuracy = float
      shortedge = float
   }
}
```

The `accuracy` parameter indicates the deviation of a structure from its original location. The default is `1e-8`.

The `shortedge` parameter removes short edges. All edges that are shorter than this parameter are eliminated. This parameter does not have a default value and is activated only when it has a nonzero value.

Rediscretizing the Boundary File

This section rediscretizes the boundary file by surface remeshing using the DelPSC algorithm that creates good-quality triangles on non-flat surfaces of the boundary:

```
Tools {
   DelaunaySurfaceRemeshing {
      DelPSCAccuracy = float
      DelPSCRidgeAngle = float
      DelPSCRidgeSampling = float
   }
}
```

The quality of the discretization is controlled by the following parameters:

- `DelPSCAccuracy` controls the deviation between the new curved surfaces and the original curved surfaces. The new curved surface can deviate from the original curved surface by, at most, the value of `DelPSCAccuracy`. New vertices lie exactly on the original surface, but new triangles cannot lie exactly on the original surface *unless* the original surface is flat. In general, the smaller the value of `DelPSCAccuracy` is, the smoother the new surface becomes, and the more accurate the new surface represents the original surface.
- `DelPSCRidgeAngle` is an angle computed at each edge. It is a dihedral angle between two shared faces. This parameter identifies the geometric features. Default is $95°$.
- `DelPSCRidgeSampling` discretizes the ridges and controls the size of small triangles. Default is $0.01\,\mu m$.

The DelPSC algorithm uses multithreading if `IOControls{numThreads=`*`integer`*`}` is specified.

Interpolating a Source Mesh to a Destination Mesh

This section allows interpolation from the source mesh to the destination mesh:

```
Tools {
   InterpolateMesh {
      DstMesh = "string"
      Conservative
      Extrapolate = true | false
      IgnoreMaterials
      Species {"string" "string" ...}
      SrcMesh = "string"
      Tolerance = float
   }
}
```

The `SrcMesh` parameter specifies the file name of the source mesh, and the `DstMesh` parameter specifies the file name of the destination mesh. By default, if no species is specified, all the fields in the source mesh are considered for interpolation.

If the `Conservative` option is specified, a second-order method described in [3] is used to perform the interpolation. If any species is specified inside the `Species` subsection, only those species will be interpolated. If the species is already present in the destination mesh, the values will be overwritten with new interpolated values. By default, the interpolation is performed between two identical materials, and the `IgnoreMaterials` option can be used to override this behavior.

When the boundary of the source and the destination meshes do not coincide exactly, `Extrapolate=true` (default) will perform the extrapolation by assigning the field value for the destination point from the closest point on the source mesh. For some applications, extrapolation is not wanted, in which case, set `Extrapolate=false` and set the appropriate `Tolerance` for searching for source elements that contain destination points.

Performing a 2D Slice of 3D Mesh or Boundary

This section performs a 2D slice of a 3D mesh or boundary:

```
Tools {
   Slice {
      location = (float float float)
      normal = (float float float)
   } |
   Slice {
      Direction = X | Y | Z
      Endpoint = (float float)
      Startpoint = (float float)
   }
}
```

NOTE The `Slice` operation applies to both the mesh and boundary.

The 2D slice is defined by a plane normal and a location (see Slicing a 3D Mesh Using a Plane and Its Location on page 99).

Alternatively, the slice can be obtained by restricting a plane by a segment. For this interface, a direction parameter indicating the plane in which the segment lies, and a starting point and an endpoint of a segment are needed. The starting point and endpoint are represented by only two coordinates of the segment, and the third coordinate is computed from the input structure. For example, if the direction is the z-plane, the coordinates of `Startpoint` and `Endpoint` represent the x- and y-values of the segment. If the direction is the y-plane, the coordinates of `Startpoint` and `Endpoint` represent the x- and z-values of the segment. Similarly, if the direction is the x-plane, the coordinates of `Startpoint` and `Endpoint` represent the y- and z-values of the segment.

Cutting a Mesh With a Plane

This section cuts a mesh with a plane:

```
Tools {
   Cut {
      normal = (float float float)
      location = (float float float)
   }
}
```

The mesh that is to the right of the plane is removed. The right side of the plane is defined as the one to which the normal points.

NOTE This operation is limited to 3D meshes and 3D boundaries. For hybrid meshes, cutting through elements will result in significant topological changes around the cutplane.

Reflecting a Mesh

This section mirrors a mesh about a location and appends it to the original mesh:

```
Tools {
   Reflection {
      axis = xmin | ymin | zmin | xmax | ymax | zmax
      map "stringA" = "stringB"
   }
}
```

NOTE This operation is limited to meshes.

The `map` statement specifies the name that corresponds an input region to the mirrored region. By default, if `map` is not specified, the new region names are given the `_mirrored` file extension.

Sweeping a Mesh

This section creates a 3D mesh from a 2D mesh by sweeping the mesh in the normal direction:

```
Tools {
   Sweepmesh {
      extension = float
      steps = integer
```

```
   }
}
```

The amount of the sweep is defined by `extension`. The `steps` parameter denotes the number of divisions that the swept mesh is divided into, in the normal direction.

Stretching a Mesh

This section stretches an existing mesh by adding a new column of elements at the specified location in the specified direction:

```
Tools {
   Stretch {
      direction = X | Y | Z
      length = float
      location = (float float float)
   }
}
```

The unit of length is the same as that of the input mesh. A negative length indicates a stretch in the opposite direction. This operation is limited to meshes.

Placing Individual Dopant of Species

This section allows you to place an individual dopant of a species at a specified location:

```
Tools {
   Dopants {
      Species "string" {
         DopantLocation = (float float float)
         ...
         DopantLocation = (float float float)
         Replace
      }
   }
}
```

If the specified location matches the mesh point, the discrete dopant will be assigned to that particular point or it will snap to the nearest mesh point. By default, the specified dopants for each species are added to the input continuous doping. If you specify the `Replace` option, the input continuous doping is reinitialized to zero for a user-specified species only in those regions that contain the specified single dopants. The other species of this region are untouched.

For example, if you specify single dopants of `BoronActiveConcentration` with the `Replace` option, only the input `BoronActiveConcentration` of the region that contains these single dopants is reinitialized to zero, and the contribution from single dopants is considered in that region. The other species of this region are untouched.

Extracting Boundary From a Mesh

You can specify the `Mesh2bnd` option to extract a boundary from a mesh, or you can set the geometric accuracy and short edge to clean up unwanted small features of the input geometry:

```
Tools {
   Mesh2bnd |

   Mesh2bnd {
      accuracy = float
      shortedge = float
   }
}
```

The default value of `accuracy` is `1e-8` µm. The geometric accuracy cleans up the coplanar mesh points. By default, this operation does not remove the short edges.

Converting a Tetrahedral Mesh to a Hybrid Mesh

Hybrid meshes (also referred to as mixed-element meshes) contain hexahedra, prisms, pyramids, and tetrahedra. They are used in some tools such as Sentaurus Device because, compared to tetrahedral meshes, hybrid meshes have fewer elements, thereby allowing the tools to perform simulations on larger structures. Hybrid meshes are also used in Sentaurus Interconnect to increase the accuracy of the simulation.

The `Mesh2Hybrid` option converts an input mesh containing only tetrahedral elements to a hybrid mesh:

```
Tools {
   Mesh2Hybrid
}
```

NOTE Sentaurus Mesh cannot use hybrid meshes directly as input for any operation specified in the `Tools` section.

NOTE When the `Mesh2Hybrid` option is processed, the output is written out directly, thereby ignoring the operations that follow in the `Tools` section.

Specifying Algorithm for Smoothing Noise

This section uses a multimaterial level-set (MLS) algorithm to smooth any noise that may be present in the boundary file:

```
Tools {
   MultiLevelSetBrepFilter {
      CellSize = float
      numThreads = integer
   }
}
```

The output of this section may contain a large number of poor-quality triangles on non-flat surfaces. You should use the `DelaunaySurfaceRemeshing` section afterwards to eliminate poor-quality triangles (see Rediscretizing the Boundary File on page 55).

The `CellSize` parameter specifies the level-set cell size, which should be, at most, one-third the thickness of the thinnest region. Otherwise, the thin region may be considered noise and it disappears. The coarser the cell size, the more features may be smoothened. Default is $0.001\ \mu m$.

The amount of geometry smoothing performed by the MLS algorithm depends on both curvatures in the input and the level-set cell size. A noisy surface has a high curvature, so it will be smoothed to a large extent to remove noise. On the other hand, a planar surface has zero curvature, so it will be well preserved. Unfortunately, a sharp corner has a theoretically infinite curvature, so it will become a rounded corner. The specified level-set cell size is the threshold to distinguish between the noise to be removed and the features to be preserved.

The `numThreads` parameter specifies the number of threads to use. Default is 1.

Creating Structures With Randomized Doping Profiles

This section creates structures with randomized doping profiles based on an original structure obtained from process simulation or created analytically. The section works by *atomizing* the original continuous doping distribution to create discrete dopants and then reassigning the doping associated with these discrete dopants back to the surrounding mesh nodes. Different atomizations or randomized structures can be obtained from one original structure.

NOTE This section does not change the mesh but reassigns the randomized doping.

The syntax is:

```
Tools {
   RandomizeDoping {
      ContinuousContactDoping
      DopingAssignment = "Sano" | "CIC" | "NGP"
      FileIndex = integer
      NumberOfRandomizedProfiles = integer
      SaveDiscreteDopants

      Material "Material name 1" {
         Species "Dataset name 1" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
         Species "Dataset name 2" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
         ...
      }

      Material "Material name 2" {
         Species "Dataset name 1" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
         Species "Dataset name 2" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
         ...
      }

      Region "Region name 1" {
         Species "Dataset name 1" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
         Species "Dataset name 2" {
            Ignore | Randomize
            ScreeningFactor = value
            AutoScreeningFactor
         }
```

```
        ...
      }

      Cuboid [ (value value value) (value value value) ] {
        Species "Dataset name 1" {
          ScreeningFactor = value
          ScreeningScalingFactor = value
          AutoScreeningFactor
        }
        Species "Dataset name 2" {
          ScreeningFactor = value
          ScreeningScalingFactor = value
          AutoScreeningFactor
        }
        ...
      }
      ...
    }
  }
```

where:

`ContinuousContactDoping`

Specifying this option discards the randomized doping assigned to the contact nodes and, instead, it uses the contact doping obtained from the original structure.

`DopingAssignment = "Sano" | "CIC" | "NGP"`

Specifies the method used to assign doping from the discrete dopants created during atomization to the mesh nodes:

- The cloud-in-cell (`"CIC"`) method distributes the doping of a particle to the vertex nodes of the element in which the particle is located.
- The nearest grid point (`"NGP"`) method assigns the doping of a particle to the nearest mesh node.
- The `"Sano"` method uses a doping function described in Appendix B on page 123 to distribute the doping of a particle to surrounding nodes.

`FileIndex (0)`

Specifies the name of output files and also is used as a random seed during randomization. The names of output files are created automatically using the following convention:

```
<root>_<DopingAssignment><FileIndex + Randomized_Profile_Number>_msh.tdr
```

where `<root>` is a base name of the input TDR file.

For example, if `DopingAssignment = "Sano"`, `FileIndex = 1000`, and `NumberOfRandomizedProfiles = 3`, and the command line is:

```
snmesh nmos
```

then the following output files are created:

```
nmos_sano1000_msh.tdr
nmos_sano1001_msh.tdr
nmos_sano1002_msh.tdr
```

`NumberOfRandomizedProfiles (1)`

Specifies the number of randomized profiles to be generated.

`SaveDiscreteDopants`

This option saves active discrete dopants along with the randomized dopant profiles. The active discrete dopants can be visualized as well as the mesh. This file also can be specified as a `ParticleFile` in the particle profile section of the `Definitions` section (see Defining Particle Profiles on page 17).

`Ignore | Randomize`

Two choices are provided for each specified species. By default, all specified species are randomized. With the `Ignore` option, a species is not randomized and is not copied to the output file. All species that are not specified in the command file for a specified material are copied to the output file.

In the `RandomizeDoping` section, only materials that are specified in the command file will have their doping randomized. Materials found in the input structure that are not specified in the command file will have their original continuous doping written to the output file. If a species is not specified for a material, it is simply copied to the output without randomizing.

For example, if the input structure contains the material `"Silicon"` with the species `"ArsenicActiveConcentration"` and `"BoronActiveConcentration"`, and the command file only specifies `"BoronActiveConcentration"`, the randomized species `"BoronActiveConcentration"` and original `"ArsenicActiveConcentration"` will contribute to the silicon doping in the final output structure.

The `ScreeningFactor` parameter and the `AutoScreeningFactor` option are used only with `DopingAssignment = "Sano"`. If `"Sano"` is selected, `ScreeningFactor` must be specified. The `AutoScreeningFactor` calculation is invoked only if specified.

In addition to materials, randomization can be restricted solely to a region or a cuboid.

NOTE When the `RandomizeDoping` section is processed, the output is written out directly, thereby ignoring the operations that follow in the `Tools` section.

Adding or Removing Interfaces From a Mesh

Some TCAD Sentaurus tools produce meshes that contain an explicit description of the interface between adjacent regions. This description is not understood by some tools and is not produced by other tools, so it is sometimes necessary to add or remove it from a mesh file.

You can specify either the `addInterfaceRegions` or the `removeInterfaceRegions` option to add interfaces or to remove interfaces, respectively.

The syntax is:

```
Tools {
   addInterfaceRegions | removeInterfaceRegions
}
```

QualityReport Section

The `QualityReport` section is optional and is used to specify mesh quality limits for mesh generation. Sentaurus Mesh produces a report regardless of whether the limits are satisfied or not. This section of the command file can help to ensure that the mesh is suitable for device simulation.

NOTE The `QualityReport` section applies only to 3D axis-aligned meshes and 3D offsetting meshes. The specified limits are used only to report on the mesh quality and do not affect how meshes are generated.

If any limits are not satisfied, Sentaurus Mesh saves additional field variables in the output `_msh.tdr` file:

- `AngleElements`: The angle of an element as defined by the box method.
- `DelaunayInsphere3D`: The number of elements that are non-Delaunay elements.
- `ElementsPerVertex`: The number of elements that share a vertex.
- `ElementVolume`: The volume of an element.
- `ShortestEdge`: The length of the shortest edge of an element.

The syntax of this section is:

```
QualityReport {
   Global
   Material = {stringList}
   Region = {stringList}
   {
      limitMaxConnectivity = integer
      limitMaxNonDelaunay = float
      limitMinAngle = float
      limitMinEdgeLength = float
      limitMinVolume = float
   }
}
```

where (default values are given in parentheses if applicable):

`Global`

If specified, the limits are evaluated on the entire mesh.

`Material`

If specified, the limits are evaluated on the list of materials only.

`Region`

If specified, the limits are evaluated on the list of regions only.

`limitMaxConnectivity (0)`

Specifies the maximum number of elements that can share any vertex. If this limit is exceeded, Sentaurus Mesh saves the `ElementsPerVertex` field variable in the output mesh file. The default value of `0` means this parameter has no effect.

`limitMaxNonDelaunay (100.0)`

Specifies the maximum percentage of all elements that can be non-Delaunay elements. If this limit is exceeded, Sentaurus Mesh saves the `DelaunayInsphere3D` field variable in the output mesh file.

`limitMinAngle (0.0)`

Specifies the minimum angle (given in degrees), defined using the box method, of any element. If this limit is exceeded, Sentaurus Mesh saves the `AngleElements` field variable in the output mesh file. See Utilities User Guide, AngleElements on page 32.

`limitMinEdgeLength (0.0)`

Specifies the minimum edge length (given in μm) of any element. If this limit is exceeded, Sentaurus Mesh saves the `ShortestEdge` field variable in the output mesh file.

`limitMinVolume (0.0)`

Specifies the minimum volume (given in μm^3) of any element. If this limit is exceeded, Sentaurus Mesh saves the `ElementVolume` field variable in the output mesh file.

Examples

Generate a report on the mesh quality of the entire mesh using the default limits:

```
QualityReport {
   Global
}
```

Generate a report on the mesh quality of the entire mesh using the default limits, followed by a report on the mesh quality of the materials `Silicon` and `Oxide` using the default limits:

```
QualityReport {
   Global
   Material = {"Silicon" "Oxide"}
}
```

Generate a report on the mesh quality of the entire mesh using the default limits, followed by a report on the mesh quality of the regions `Substrate` and `Oxide_1` using the default limits:

```
QualityReport {
   Global
   Region = {"Substrate" "Oxide_1"}
}
```

Generate a report on the mesh quality of the entire mesh with two specific limits:

```
QualityReport {
   Global {
      limitMaxNonDelaunay = 0.1
      limitMinAngle = 1e-2
   }
}
```

Generate a report on the mesh quality of the entire mesh with one set of limits, followed by a report on the mesh quality of the material `Silicon` with a different set of limits:

```
QualityReport {
   Global {
      limitMaxNonDelaunay = 0.1
      limitMinAngle = 1e-2
```

```
    }
    Material = {"Silicon"} {
       limitMinVolume = 1e-18
       limitMinEdgeLength = 1e-5
    }
}
```

References

[1] S.-W. Cheng, T. K. Dey, and J. A. Levine, “A Practical Delaunay Meshing Algorithm for a Large Class of Domains,” in *Proceedings of the 16th International Meshing Roundtable*, Seattle, WA, USA, pp. 477–494, October 2007.

[2] T. K. Dey and J. A. Levine, “Delaunay Meshing of Piecewise Smooth Complexes without Expensive Predicates,” *Algorithms*, vol. 2, no. 4, pp. 1327–1349, 2009.

[3] F. Alauzet and M. Mehrenberger, “P^1-conservative solution interpolation on unstructured triangular meshes,” *International Journal for Numerical Methods in Engineering*, vol. 84, no. 13, pp. 1552–1588, 2010.

CHAPTER 3 Doping and Refinement Examples

This chapter illustrates how to use the Definitions and Placements sections of the command file, as well as how to use the Offsetting section to generate layered meshes in Sentaurus Mesh.

Command File for a Simple Diode

This section describes the command file `diode.cmd` that is used as an example for the rest of this chapter. The command file contains two types of information: dimension-independent data and dimension-dependent data. The dimension-independent part of the command file `diode.cmd`, for this example, is:

```
Title "minimal example: simple diode"
Definitions {
   # Profiles
   Constant "n-type region" {
      Species = "PhosphorusActiveConcentration" Value = 1e+18
   }
   Constant "p-type region" {
      Species = "BoronActiveConcentration" Value = 1e+17
   }
}
```

The optional keyword `Title` is used for a short description of the device and mesh. The `Definitions` section specifies the dimension-independent part of the command file and can be used for all dimensions without modifications.

Two constant profiles for doping are described using the keyword `Constant` followed by the profile name in double quotation marks. The keyword `Species` is used to declare the doping species used in the region. The constant concentration is specified by the number following the keyword `Value`. The sign is intrinsic to the species.

Now, the doping profiles must be placed in the device. The placement of these profiles depends on the device geometry. Since, for this example, ‘solid’ regions are to be filled with constant doping, these instructions are added to the command file:

```
Placements {
   # Profiles
   Constant "n-type region instance" {
      Reference = "n-type region"
      EvaluateWindow {
```

```
            Element = cuboid [(1 0 0), (2 3 2)]   # for 3D
         }
      }
      Constant "p-type region instance" {
         Reference = "p-type region"
         EvaluateWindow {
            Element = cuboid [(0 0 0), (1 3 2)]   # for 3D
         }
      }
   }
```

The keyword `Placements` starts the dimension-dependent section where the instances of the definitions given in the `Definitions` section are defined. The `Reference` parameter specifies a profile defined in the `Definitions` section. The `EvaluateWindow` defines the valid domain for the profiles. In this example, the valid domains are lines in 1D, rectangles in 2D, and cuboids in 3D. If `EvaluateWindow` is not defined in the file, the profile is valid in the entire domain of the device.

For the 3D case, the valid domain of the p-type region is the lower half of the device, given by the cuboid [(0 0 0), (1 2 3)]. In 2D, this domain is given by the rectangle [(0 0), (1 2)] and in 1D, by the line [(0), (1)]. However, the doping profile defined for 3D can be used for the lower dimensions and, for the rest of this chapter, only the command file for the 3D case will be used.

In the example, there is an abrupt decay function between the two constant profiles. The doping associated with points outside the `EvaluateWindow` is zero. This situation can be modified if the parameter `DecayLength` is used. By setting `DecayLength` in `EvaluateWindow`, an error function can be used as a decay profile.

Refinement and Evaluation Windows

The refinement conditions specified inside a `Refinement` statement can be restricted using refinement windows. The windows can be simple rectangles, polygons, polyhedra, regions, or materials.

Using Refinement Polygons

Figure 1 on page 72 illustrates the use of polygonal domains for specifying a polygonal `RefineWindow` and for using a polygonal domain as an `EvaluateWindow`. The domain is a simple rectangular boundary and the command file is:

```
Title "Refinement Polygon"
Definitions {
   Refinement "global" {
```

```
      MaxElementSize = (4, 4)
      MinElementSize = (.04 .04)
      RefineFunction = MaxTransDiff(Variable="DopingConcentration", Value=0.5)
   }
   Refinement "refpol" {
      MaxElementSize = (0.3 0.1)
   }
   Constant "bor" {
      Species = "BoronConcentration" Value=1e+17
   }
}

Placements {
   Refinement "global" {
      Reference = "global"
      RefineWindow = rectangle [( -2 -2 ), ( 14 14 )]
   }
   Refinement "refpol" {
      Reference = "refpol"
      RefineWindow = polygon [( 1 2 ) ( 0.75 2 ) ( 1 2.5 ) ( 1.25 3 )
      ( 1.5 3.5 ) ( 1.75 4 ) ( 2 4.25 ) ( 2.25 4.5 ) ( 2.5 4.75 ) ( 2.75 5 )
      ( 2.75 5.5 ) ( 3 5.75 ) ( 3.5 5.5 ) ( 4 5.75 ) ( 4.5 5.5 ) ( 5 5.5 )
      ( 5.5 5.75 ) ( 5.5 6 ) ( 6 6.25 ) ( 6.5 6 ) ( 7 6 ) ( 7.5 5.25 )
      ( 8 5.5 ) ( 8 5 ) ( 7.5 4.5 ) ( 8 4.25 ) ( 8.5 4 ) ( 9 3.75 ) ( 9.5 4 )
      ( 9.5 3.5 ) ( 9.5 3 ) ( 9 3 ) ( 8.5 2.75 ) ( 8.75 2.5 ) ( 8.5 2.25 )
      ( 8 2.25 ) ( 7.5 2.25 ) ( 7.5 2.5 ) ( 7 2.5 ) ( 7 2 ) ( 6.75 1.5 )
      ( 6.75 1 ) ( 6.25 1  ) ( 6 1.5 ) ( 5.5 2  ) ( 5.5 2.5 ) ( 5 2 )
      ( 4.75 1.5 ) ( 4.5 1 ) ( 4 1.25 ) ( 3.5 1.25 ) ( 3 1 ) ( 2.5 1.5 )
      ( 2.5 2 ) ( 2.5 2.5 ) ( 2 2.5 ) ( 1.5 2.5 ) ( 1.5 2 ) ( 1 2 )]
   }
   Constant "bor" {
      Reference = "bor"
      EvaluateWindow {
         Element = polygon [( 1 2 ) ( 0.75 2 ) ( 1 2.5 ) ( 1.25 3 ) ( 1.5 3.5 )
         ( 1.75 4 ) ( 2 4.25 ) ( 2.25 4.5 ) ( 2.5 4.75 ) ( 2.75 5 )
         ( 2.75 5.5 ) ( 3 5.75 ) ( 3.5 5.5 ) ( 4 5.75 ) ( 4.5 5.5 ) ( 5 5.5 )
         ( 5.5 5.75 ) ( 5.5 6 ) ( 6 6.25 ) ( 6.5 6 ) ( 7 6 ) ( 7.5 5.25 )
         ( 8 5.5 ) ( 8 5 ) ( 7.5 4.5 ) ( 8 4.25 ) ( 8.5 4 ) ( 9 3.75 )
         ( 9.5 4 ) ( 9.5 3.5 ) ( 9.5 3 ) ( 9 3 ) ( 8.5 2.75 ) ( 8.75 2.5 )
         ( 8.5 2.25 ) ( 8 2.25 ) ( 7.5 2.25 ) ( 7.5 2.5 ) ( 7 2.5 ) ( 7 2 )
         ( 6.75 1.5 ) ( 6.75 1 ) ( 6.25 1 ) ( 6 1.5 ) ( 5.5 2 ) ( 5.5 2.5  )
         ( 5 2  ) ( 4.75 1.5 ) ( 4.5 1 ) ( 4 1.25 ) ( 3.5 1.25 ) ( 3 1 )
         ( 2.5 1.5 ) ( 2.5 2 ) ( 2.5 2.5 ) ( 2 2.5 ) ( 1.5 2.5 ) ( 1.5 2 )
         ( 1 2 )]
      }
   }
}
```

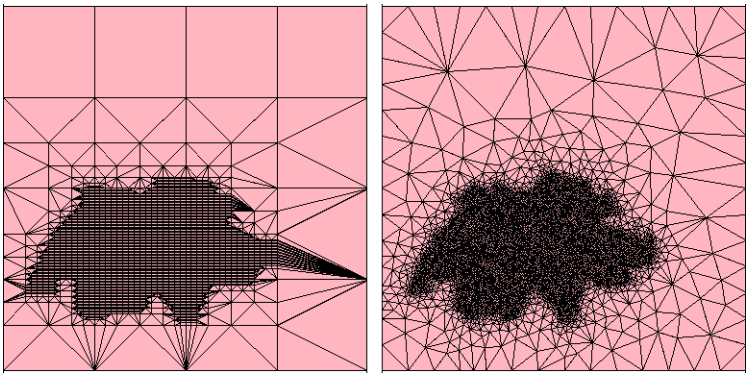


Figure 1 Polygonal refinement

Using Composite Elements

Geometric elements can be combined to form more complex elements. This can be used to define curved reference elements for analytic profiles, which otherwise cannot be correctly defined using the standard elements. An example of the use of a composite element is:

```
AnalyticalProfile "MyProfile" {
   Reference = "MyProfileReference"
   ReferenceElement {
      Element = {
         line [( -1 2 ) , ( 4 2 )]
         line [( 4 2 ) , ( 6 4 )]
         line [( 6 4 ) , ( 7 4 )]
      }
   }
}
```

NOTE For the composite element to be effective, all components must be adjacent to each other, without leaving gaps between them.

NOTE Composite elements are available only in Sentaurus Mesh.

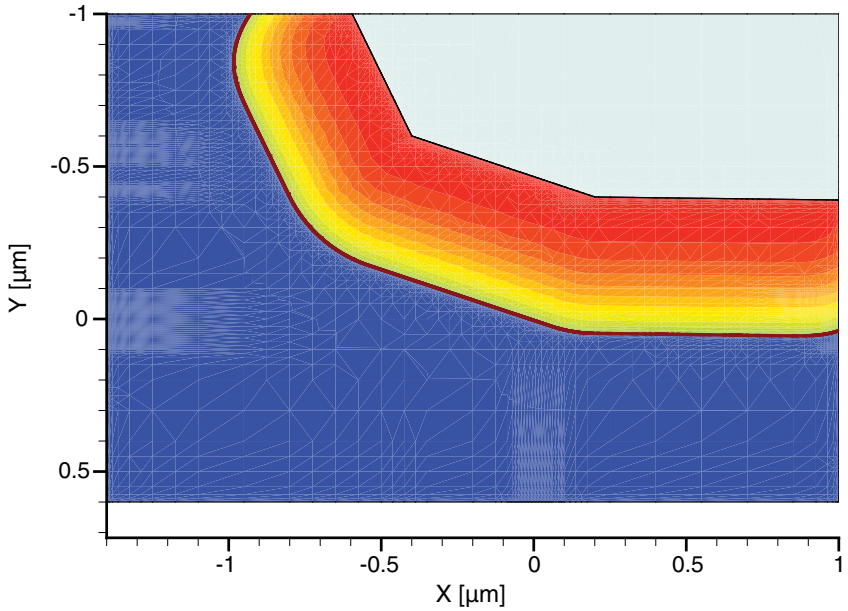


Figure 2 Profile built by combining several reference elements

Regionwise and Materialwise Refinement

Figure 3 on page 74 illustrates the effect of using regionwise and materialwise refinement. The following command file segment shows the relevant part of the command file:

```
Placements {
   Refinement "A" {
      Reference = "A"
      RefineWindow = region ["Ox_Region"]
   }
   Refinement "B" {
      Reference = "B"
      RefineWindow = material ["Oxide"]
   }
}
```

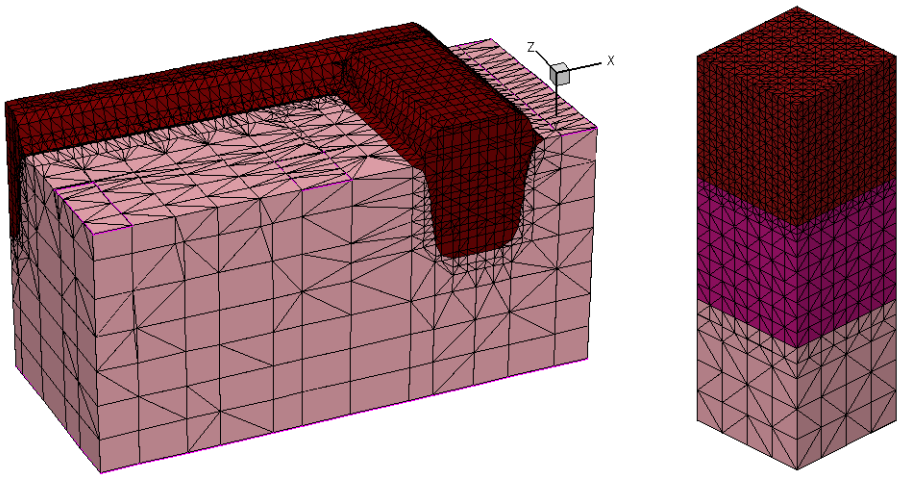
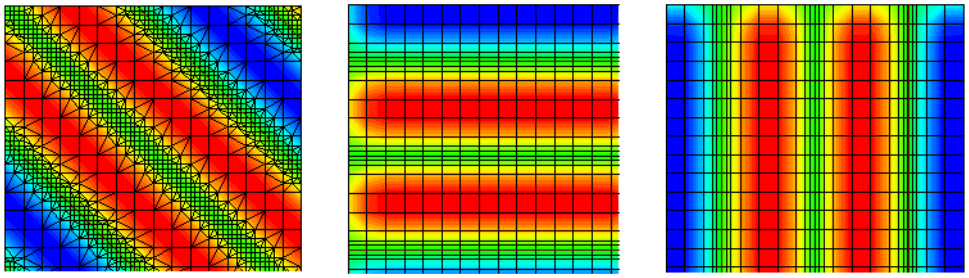


Figure 3 (*Left*) Regionwise and (*right*) materialwise refinement

Using Analytic Functions for Doping Specification

This example illustrates the use of general analytic functions for defining doping profiles. To use the primary and lateral directions as x and y, the keyword `Eval` must be specified (instead of `General`), that is, by using global spatial coordinates. Figure 4 shows the generated meshes.

```
AnalyticalProfile "NoName_0" {
   Species = "BoronActiveConcentration"
   Function = Eval(init="a=10",function = "a*sin(x)*cos(y)",value = 0)
}
ReferenceElement {
   Element = line [( 0 0 ), ( 10 10 )]
   # Element = line [( 0 5 ), ( 10 5 )]
   # Element = line [( 5 0 ), ( 5 10 )]
}
```



Element=line[(0 0),(10 10)] Element=line[(0 5),(10 5)] Element=line[(5 0),(5 10)]

Figure 4 Use of analytic refinement functions for doping

Creating 3D Profiles From 2D Cross Sections

A 2D profile can be extended into three dimensions by using an `EvaluateWindow` containing a `sweepElement`, which is an advanced type of element that allows a 2D geometric element to be either swept along a path or swept about a reference axis.

A `sweepElement` is composed of a base element, which can be either a polygon or a rectangle, and a path, which can be represented in several ways. When a 3D profile is evaluated, the `sweepElement` takes the 3D coordinate and follows the path in reverse, calculating a local 2D coordinate on the base element. This 2D coordinate is then used to evaluate the 2D profile and to provide the values in 3D.

NOTE A `sweepElement` can be used only in `EvaluateWindow` statements. Using it in a `ReferenceElement` or `RefinementWindow` statement will generate error messages.

To sweep a 2D profile along a path, use the one of the following syntax templates:

```
# Sweep the base element a distance along the normal to the element.
sweepElement {
   base = <2D Element>
   distance = <double>
}

# Sweep the base element along a vector. The vector must be
# normal to the base element.
sweepElement {
   base = <2D Element>
   vector = (x1,y1,z1)
}

# Sweep the base element along a polygonal path. The origin of
# the path must be normal to the base element.
sweepElement {
   base = <2D Element>
   path = [(x1,y1,z1)...(xn,yn,zn)]
}

# Rotate the base element about an axis parallel to the z-axis.
# The axis will be placed at the center of the base element.
sweepElement {
   base = <2D Element>
   angle = <double>
}

# Rotate the base element about an axis parallel to the z-axis
# which is placed at a point "p".
```

```
sweepElement {
   base     = <2D Element>
   point    = p
   angle    = <double>
}

# Rotate the base element about an axis.
sweepElement {
   base     = <2D Element>
   point    = (x,y,z)
   axis     = (dx,dy,dz)
   angle    = <double>
}
```

In some cases, the normal of the base element is used to determine the direction of the sweep. This normal is calculated in the following way:

- For a polygonal base element described using the sequence $[p_1, p_2, \ldots, p_n]$, the normal is calculated as $(p_3 - p_2) * (p_1 - p_2)$.
- For a rectangular base element described by $[p_1, p_2]$, the normal calculation is extremely complicated and is not described here. The recommendation is to use polygonal elements, or to swap p_1 and p_2 if the profile is being produced in the wrong direction.

More considerations arise when rotating an element about an axis (see Figure 5). Since there are some degrees of freedom to perform the rotation, additional rules must be applied:

- Only the right side of the profile is used in the sweep. This is to avoid double-defined values, which occur when the rotation axis is contained inside the base element and the rotation angle is more than $180°$.
- The direction of the rotation is adjusted to match the direction of the normal.

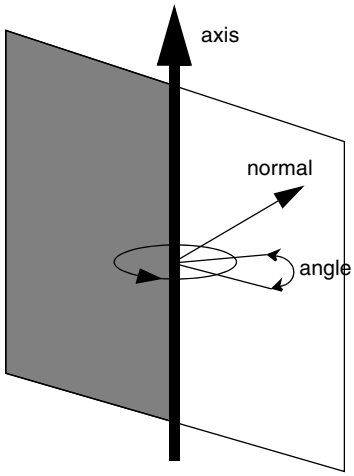


Figure 5 Rotation of a profile about an axis; the gray portion is ignored during the sweep

The angle can be set to a negative value, or the orientation of the axis can be reversed, to obtain the required profile.

When a 2D submesh profile is loaded into a 3D simulation, the default is to place it along the xy coordinate plane. The `ShiftVector` and `Rotation` parameters must be used to place the profile at the desired location.

For example, to place a submesh on the xz plane, passing through the point (0, 50, 50), and then to sweep it along a path, the following can be used:

```
SubMesh "profile" {
   Reference = "SubMesh"
   Rotation {
      angle = -90
      axis = X
   }
   ShiftVector = (0 50 50)
   EvaluateWindow {
      Element = sweepElement {
         base = rectangle [(0 45 0), (15 45 50)]
         path = [(15 45 0) (15 35 0) (30 45 0) (35 25 0)]
      }
      DecayLength = 1
   }
}
```

Using Particle Profiles to Specify Doping

This example illustrates the use of particle profiles for specifying the doping for a 30-nm n-channel MOSFET. The particle information is generated by Sentaurus Process Kinetic Monte Carlo and is stored in a TDR file named `30nm_end6.tdr`. Figure 6 on page 78 shows the results of the kinetic Monte Carlo (KMC) simulation with the gate material and gate oxide removed. The light blue dots represent arsenic point defects, and the dark blue dots represent boron point defects.

The command file `nmos.cmd` shown below is used to generate the mesh and doping for the structure.

NOTE Before running `nmos.cmd`, a 3D boundary file named `nmos_bnd.tdr` should exist that is consistent with the KMC particle file. If the final generated structure is to be used in Sentaurus Device, the boundary file must also contain the proper electrodes needed for device simulation.

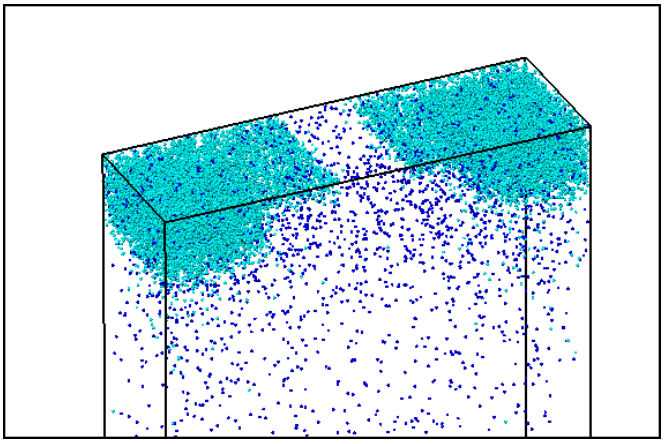


Figure 6 Discrete dopant positions generated by Sentaurus Process Kinetic Monte Carlo

The `Definitions` section of the command file defines the profiles and refinements that will later be used (in the `Placements` section) to create the mesh and doping for the structure:

```
Title "Specifying doping with particle profiles"
Definitions {
   Constant "PolyGateDoping" {
      Species = "ArsenicActiveConcentration"
      Value = 8e+19
   }
   Particle "BoronParticles" {
      ParticleFile = "30nm_end6.tdr"
      Species = "BoronActiveConcentration"
      ScreeningFactor = 2.5e6
      AutoScreeningFactor
      Normalization
   }
   Particle "ArsenicParticles" {
      ParticleFile = "30nm_end6.tdr"
      Species = "ArsenicActiveConcentration"
      ScreeningFactor = 1.0e7
      AutoScreeningFactor
      Normalization
   }
   Refinement "GlobalRefinement" {
      MaxElementSize = ( .020 .020 .020 )
      MinElementSize = ( .002 .002 .002 )
      RefineFunction = MaxTransDiff(Variable = "DopingConcentration",Value = 1)
   }
   Refinement "InterfaceRefinement" {
      MaxElementSize = ( .008 .004 .0002 )
      MinElementSize = ( .002 .002 .0001 )
```

```
      RefineFunction = MaxTransDiff(Variable = "SpatialCoordinates",
         Value = 1e-10)
   }
}
```

The `Constant` definition defines the doping that will be used for the polysilicon gate. Two `Particle` profiles are used to obtain separately the boron and arsenic discrete dopants from the KMC particle file. Separate `ScreeningFactor` values are specified for these two `Species`. Specifying `AutoScreeningFactor` generally results in a smoother and more accurate final profile in structures where there are large changes in dopant density. The `Normalization` option compensates for doping loss of dopants located near the boundary. The command file also includes a global refinement definition based on doping and an interface refinement definition based on spatial coordinates. The latter definition is intended to force a grid refinement using the specified element sizes.

The `Placements` section of the command file specifies how the profile and refinement definitions should be used to create the structure:

```
Placements {
   Constant "PolyGateDopingPlacement" {
      Reference = "PolyGateDoping"
      EvaluateWindow { Element = material ["PolySilicon"] }
   }
   Particle "ArsenicParticlesPlacement" {
      Reference = "ArsenicParticles"
      EvaluateWindow { Element=material ["Silicon"] }
   }
   Particle "BoronParticlesPlacement" {
      Reference = "BoronParticles"
      EvaluateWindow { Element=material ["Silicon"] }
   }
   Refinement "GlobalRefinementPlacement" {
      Reference = "GlobalRefinement"
      RefineWindow = material ["Silicon"]
   }
   Refinement "InterfaceRefinementPlacement" {
      Reference = "InterfaceRefinement"
      RefineWindow = Cuboid [(0.00 0.060 0.0000) (0.05 0.090 -0.0008)]
   }
}
```

The gate material (polysilicon) is uniformly doped using the `Constant` profile given in the `Definitions` section. The `Particle` profiles are only placed in the silicon portion of the structure. The global refinement (based on doping) is also only performed in silicon. The interface refinement is confined to the channel region of the structure and to within 8 Å of the interface.

Execution of this command file will generate a TDR file named `nmos_msh.tdr`. The generated structure is shown in Figure 7.

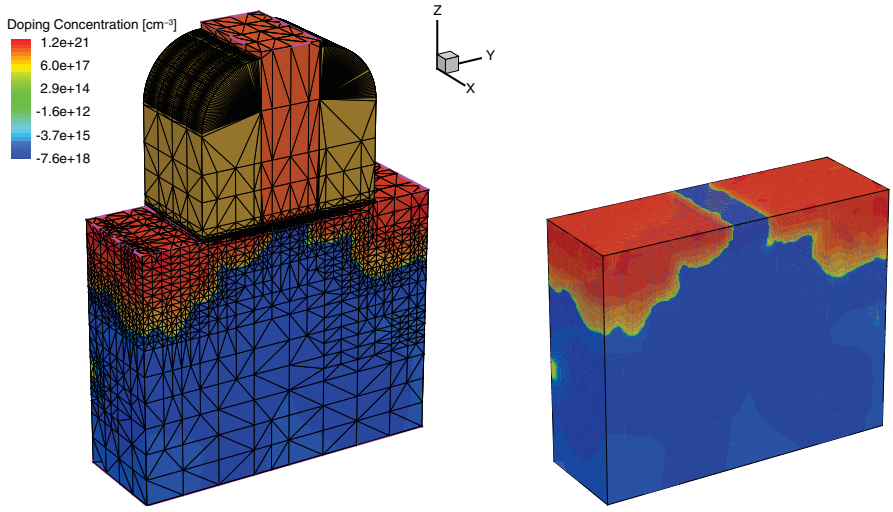


Figure 7 Mesh and doping for the structure generated by Sentaurus Mesh

Generating 2D Mesh With Continuous Doping Obtained From 3D KMC File Containing Particle Information

This example illustrates the use of the feature that generates a continuous profile on a 2D mesh from a 3D KMC file containing particle information. This feature allows you to evaluate the 3D doping profile and to transfer those onto a 2D mesh.

The following are the `Particle` subsections of the `Placements` section of the command file:

```
Placements {
   Particle "BoronParticles" {
      ParticleFile = "n26_final.tdr"
      Species = "BoronActiveConcentration"
      ScreeningFactor = 3.5e6
      AutoScreeningFactor
      Normalization
      BoundaryExtension = 0.05
      Divisions = 10
   }
   Particle "ArsenicParticles" {
      ParticleFile = "n26_final.tdr"
      Species = "ArsenicActiveConcentration"
      ScreeningFactor = 1.1e7
      AutoScreeningFactor
```

```
        Normalization
        BoundaryExtension = 0.05
        Divisions = 10
    }
}
```

The parameter boundary extension is used internally as the thickness of a 3D structure generated by extruding a 2D structure in the z-direction. The KMC file containing the particle information is mapped onto this 3D structure. For each 2D mesh point, a number of points equal to the number of divisions is created, each separated by an equal amount in the z-direction, and doping is computed on these points. The average doping is computed and is assigned to a 2D mesh point. Figure 8 shows the input boundary and generated mesh with particle profile.

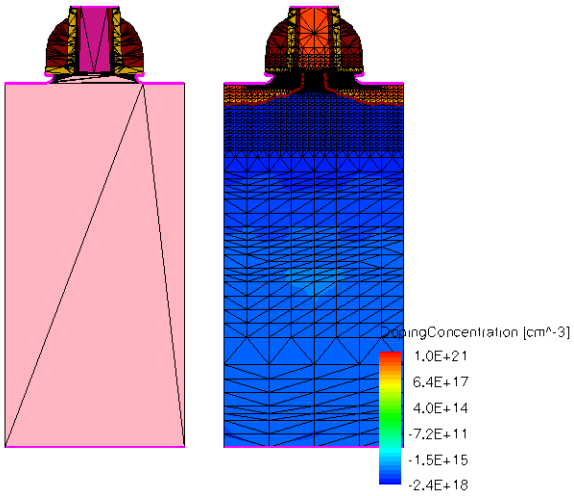


Figure 8 Two-dimensional boundary and mesh with doping obtained from a 3D KMC file

Performing Interface Refinement

Interface refinement is specified in a similar way to the refinement on analytic functions. To perform interface refinement, define a `RefineFunction` of type `MaxLengthInterface` and specify the pair of materials defining the interface, the initial thickness, and a factor used to define how this thickness should grow into the material.

The following examples illustrate the use of this function:

- This function refines silicon at the oxide interface, starting with a layer of 0.02 µm and gradually increasing the thickness by 1.4 times:

```
RefineFunction = MaxLenInt(Interface("Silicon","Oxide"), Value = 0.02,
    Factor = 1.4)
```

- This function refines all interfaces, creating a single layer of 0.01 µm:

```
RefineFunction = MaxLengthInterface(Interface("All","All"), Value=0.01)
```

- This function refines all contacts in the mesh:

```
RefineFunction = MaxLenInt(Interface("All","Contact"), Value=0.01)
```

- To refine around a single contact, specify:

```
RefineFunction = MaxLengthInterface(Interface("All","Gate"), Value=0.01,
   UseRegionNames)
```

By default, the interface refinement is performed only on the first material of the specified pair of materials describing the interface. To refine on both sides of the interface, use the `DoubleSide` keyword:

```
RefineFunction = MaxLenInt(Interface("Silicon","Contact"), Value=0.01,
   DoubleSide)
```

Ignoring Interfaces Between Regions of the Same Material

When Sentaurus Mesh performs refinement across interfaces, it internally splits the edges crossing the interfaces into segments that are contained completely inside each region. Then, it proceeds to analyze the refinement criteria on each segment independently. In some applications, the doping concentration on each region is constant, so no refinement is applied since the gradient along each segment is zero.

However, sometimes, you may want to define different doping concentrations on adjacent regions of the same material and may want the code to ignore the interface between those regions so that Sentaurus Mesh can refine across the interface. In this case, specify the parameter `skipSameMaterialInterfaces` in the `AxisAligned` section of the command file to obtain the required effect.

Offsetting Mesh Generation

This section presents examples that illustrate using the offsetting mesh generator.

Simple Example

This example shows all the relevant parameters in the `Offsetting` section that are supported by Sentaurus Mesh. The input structure is shown in Figure 9 on page 83.

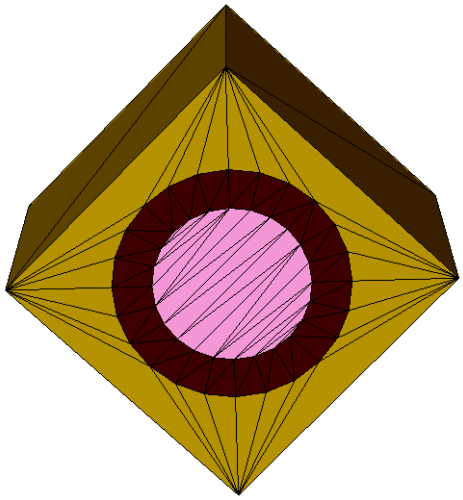


Figure 9 Simple structure

```
Title ""
IOControls {
   EnableSections
}

Definitions {
   Refinement "R5" {
      MaxElementSize = ( 0.026 0.026 0.026 )
   }
}

Placements {
   Refinement "GDJ_RP" {
      Reference = "R5"
      RefineWindow = Cuboid [(-0.2 -0.2 0) (0.20 0.2 0.5)]
   }
}

Offsetting {
   noffset {
      hlocal=0
   }
   noffset material "Silicon" {
      maxlevel = 5
   }
   noffset material "Oxide" {
      maxlevel = 5
   }
   noffset material "Silicon" "Oxide" {
      hlocal=0.002
      factor=1.5
```

```
    }
    noffset material "Oxide" "Silicon" {
       hlocal=0.002
       factor=1.5
    }
    noffset region "RTrench" "RBulk" {
       hlocal=0.002
       factor=1.5
    }
    noffset region "RBulk" "RTrench" {
       hlocal=0.002
       factor=1.5
    }
}
```

In the above command file, the global `hlocal` value is set to zero. Later, a nonzero `hlocal` value and `factor` is set using the material interface section. The default `maxlevel` value of 200 is also reset to 5 using a material section.

If the command file only includes the `Offsetting` section, without specifying any refinement criteria in the `Definitions` and `Placements` sections, the resultant mesh will be coarse as shown in Figure 10.

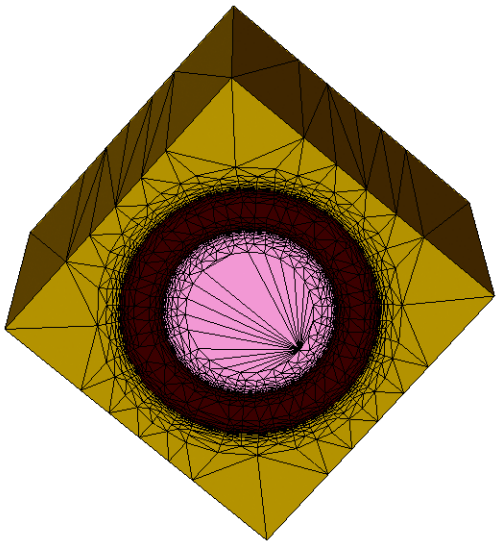


Figure 10 Coarse mesh generated with layers and without refinement criteria

With the refinement shown in the above command file, the mesh generated is shown in Figure 11.

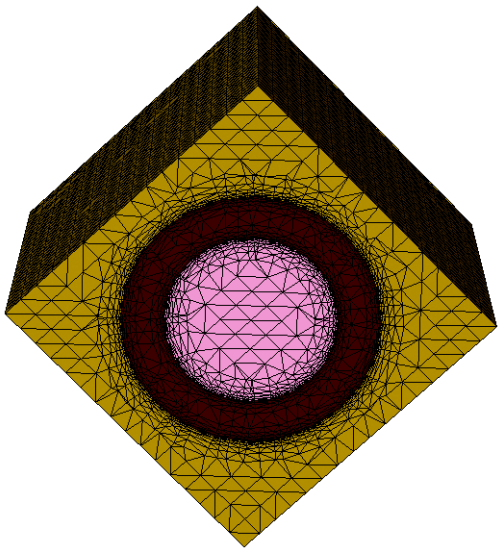


Figure 11 Mesh generated with layers along with refinement criteria

Layering From All Boundaries

```
Title ""
IOControls {
   EnableSections
}

Definitions {
   Refinement "RefinementDefinition_1" {
      MaxElementSize = ( 0.2 0.2 0.2 )
      MinElementSize = ( 0.001 0.001 0.001 )
   }
}

Placements {
   Refinement "RefinementPlacement_1" {
      Reference = "RefinementDefinition_1"
      RefineWindow = region ["R_Silicon"]
   }
   Refinement "RefinementPlacement_2" {
      Reference = "RefinementDefinition_1"
      RefineWindow = region ["R_Oxide"]
   }
}
```

```
Offsetting {
   noffset {
      hlocal=0.01
      maxlevel=6
   }
   noffset material "Oxide" "Silicon" {
      factor=2
   }
}
```

In the above command file, the global parameter `maxlevel` is set to 6 and the global `hlocal` is a nonzero value. This results in layering only from interfaces excluding exterior boundaries. If layering is required from all interfaces including boundaries that do not share any, the `Offsetting` section can be modified as shown:

```
Offsetting {
   noffset {
      maxlevel=6
   }
   noffset material "All" "All" {
      hlocal=0.01
      factor=2
   }
}
```

The string `"All"` refers to all materials in the input structure. The resultant meshes that are generated using the original `Offsetting` section and the modified `Offsetting` section are shown in Figure 12.

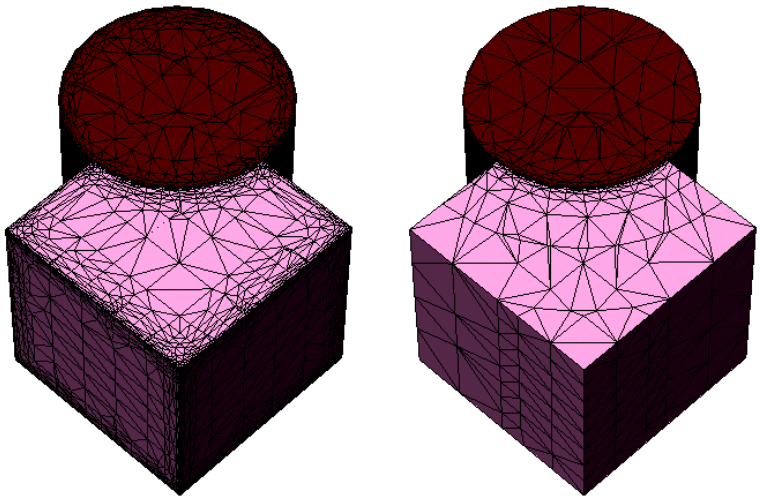


Figure 12 (*Left*) Mesh with layering from all interfaces and from boundaries with nonzero global hlocal value and (*right*) mesh generated with modified Offsetting section having layering only at interfaces

Localizing the Refinement Using Cuts

By design, the axis-aligned algorithm always creates the mesh by refining an initial box, which contains the whole device. This creates problems when the external shape of the device must be modified, because this will change the bounding box of the device, thereby altering the location of the mesh nodes.

To help resolve this situation, the axis-aligned algorithm offers the possibility of defining an initial array of boxes from which to start the refinement. This is performed through the `xCuts`, `yCuts`, and `zCuts` parameters in the `AxisAligned` section.

Each cut defines and initial refinement line that runs throughout the whole device. The boxes created with these initial lines can be refined independently of each other. Therefore, if the shape of the device changes and the cuts are adjusted accordingly, the mesh should stay the same in the sections where the boxes have remained unchanged.

The following example uses two lines to generate a total of three initial boxes. The lines are placed on either side of the channel and can be used to parameterize a set of structures where the only difference is the channel length:

```
AxisAligned {
   xCuts = (4.837 7.156)
}
```

Figure 13 displays the channel of an NMOS structure that has been refined using the standard refinement parameters.

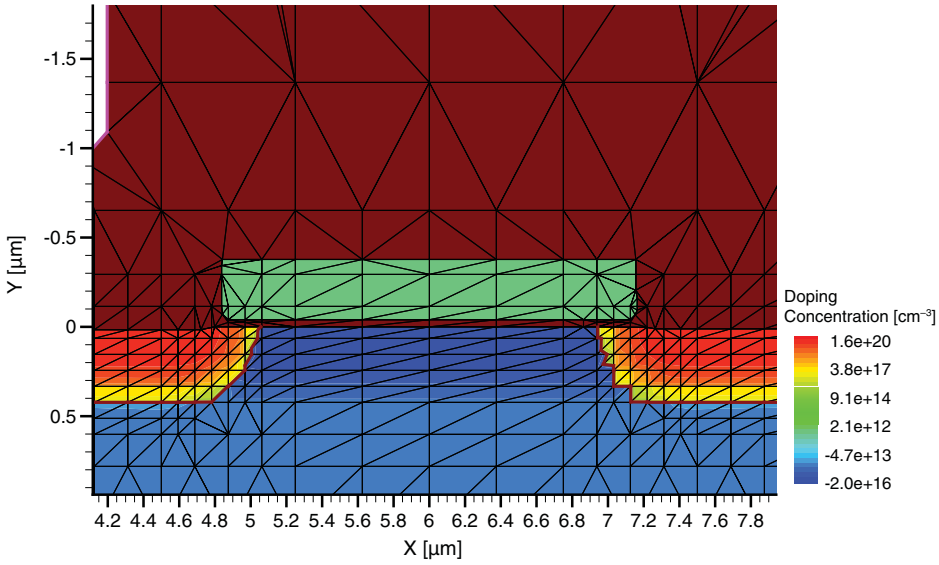


Figure 13 NMOS structure refined using standard refinement

When the `xCuts` parameter is used, two refinement lines are placed at locations x=4.837 and x=7.156 (see Figure 14). If the channel length is increased by 0.01 µm , the second x-line could be placed at 7.157, thereby preserving the mesh on either side of the channel.

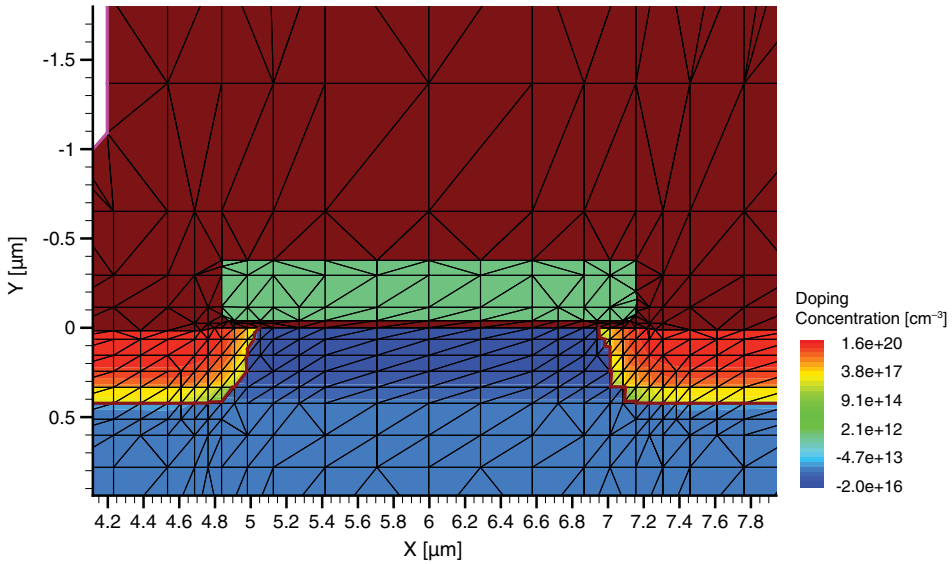


Figure 14 NMOS structure refined using the xCuts option

Another possibility is to use the `fitInterfaces` parameter in the `AxisAligned` section of the command file. This parameter works best on simple devices where all interfaces are axis aligned. Figure 15 shows that the device can be overrefined when the interfaces are not simple.

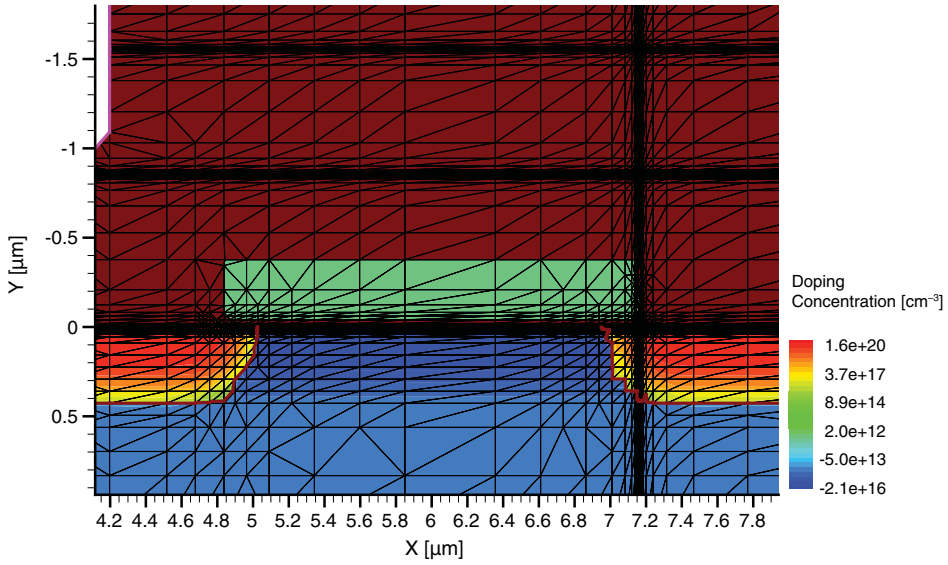


Figure 15 NMOS structure refined using the fitInterfaces parameter

Using Analytic Functions for Refinement I

Figure 16 illustrates the use of general analytic functions to specify profiles.

The function $0.1\sin(x)\sin(y)$ is used as a profile and linear interpolation (`"ElectrostaticPotential"`) is used to compute the required local element size. The following command file segment illustrates the syntax:

```
Definitions {
   Refinement "Region_1" {
      MaxElementSize = (1 1)
      MinElementSize = (0.01 0.01)
      RefineFunction = MaxTransDiff(Variable = "ElectrostaticPotential",
         Value = 0.01)
   }
   AnalyticalProfile "Profile_1" {
      Species = "ElectrostaticPotential"
      Function = General(init="a=0.1",function = "a*sin(x)*sin(y)",value = 0)
   }
}

Placements {
   Refinement "Region_1" {
      Reference = "Region_1"
   }
   AnalyticalProfile "Profile_1" {
      Reference = "Profile_1"
      EvaluateWindow {
         Element = rectangle [(0 0), (9.43 9.43)]
      }
   }
}
```

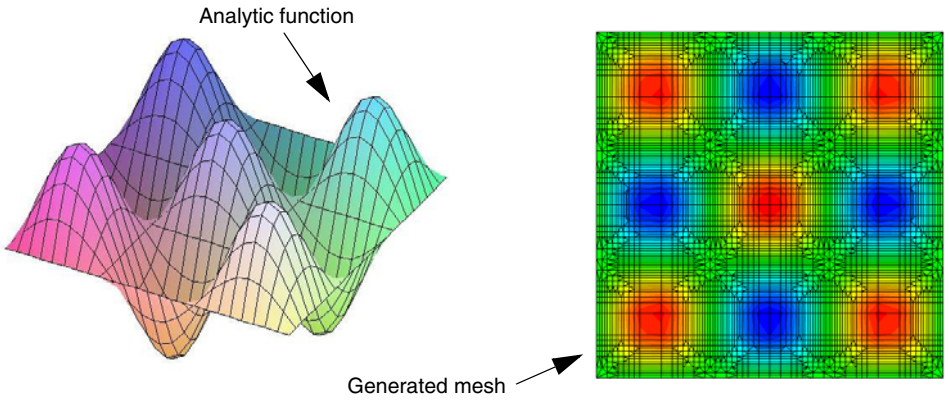


Figure 16 Use of analytic refinement functions

Using Analytic Functions for Refinement II

This example illustrates the use of a general analytic function to prescribe 3D refinement based on a 3D analytic function. The domain is a cube. Figure 17 shows the generated mesh.

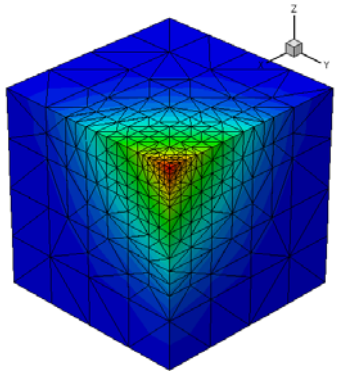


Figure 17 Use of analytic refinement functions

```
Definitions {
   Refinement "Region_1" {
      MaxElementSize = (4 4 4)
      MinElementSize = (0.01 0.01 0.01)
      RefineFunction = MaxTransDiff(Variable = "ElectrostaticPotential",
         Value = 10000.0)
   }
   AnalyticalProfile "Profile_1" {
      Species = "ElectrostaticPotential"
      Function = General(init="a=0.1",function = "a*x*x*y*y*z*z",value = 0)
   }
}

Placements {
   Refinement "Region_1" {
      Reference = "Region_1"
   }
   AnalyticalProfile "Profile_1" {
      Reference = "Profile_1"
      EvaluateWindow {
         Element = cuboid [ ( 0 0 0 ), ( 10 10 10 )]
      }
   }
}
```

CHAPTER 4 Tensor-Product Examples

This chapter uses various examples to demonstrate the applications of the Tensor section of the command file.

Simple Cube

This example illustrates the effectiveness of various features such as `maxBndCellSize`, `maxCellSize`, refinement using `window`, and `grading`. The following is the command file used to generate the tensor-product mesh:

```
Tensor {
   Mesh {
      maxBndCellSize direction "x" 0.001
      maxCellSize region "Region_0" 0.1
      window "testbox" 0.8 1.2 0.8 1.2 0.8 1.2
      minNumberOfCells window "testbox" 20
      grading = { 1.1 1.1 1.1 }
   }
}
```

Figure 18 shows the geometry of this example. In the above command file, the first parameter is `maxBndCellSize`, which is constrained in the x-direction by specifying the `direction` option. As a result, clustering is obtained only near the boundaries that are normal to the x-axis (see Figure 18, *right*).

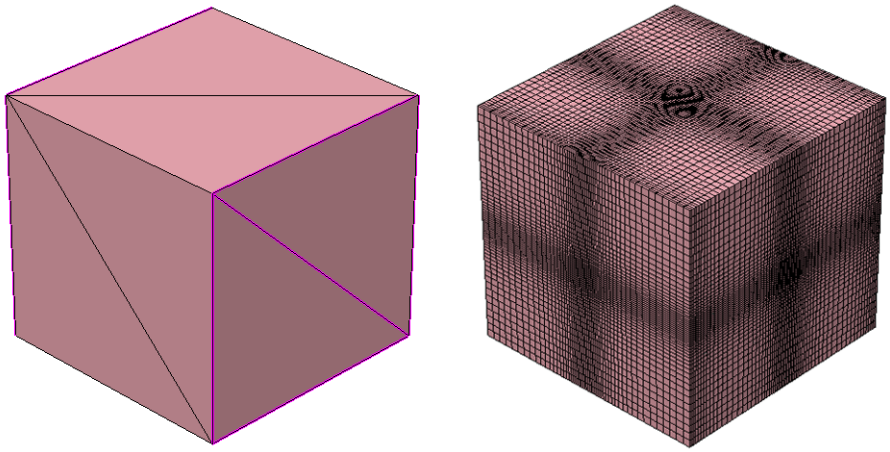


Figure 18 Geometry of a cube with a width of 2.0 units in each direction: (*left*) the input geometry and (*right*) corresponding tensor mesh

The second parameter `maxCellSize` is specified within a `region`. Since no `direction` option is used in this parameter, the mesh generator will try to obtain the same cell size in all three directions. To obtain refinement in the center of the geometry, the third parameter `window` is defined. The required refinement within a window can be obtained by specifying either `maxCellSize` or `minNumberOfCells`.

In this example, `minNumberOfCells` is used to specify the refinement. As a result of this refinement parameter, clustering of lines is visible in Figure 18 on page 91. The `grading` parameter is also defined in this command file. This is used to obtain a smooth variation of the cell sizes between various cell sizes (see Figure 19).

In Figure 18, the clustering of cells normal to the x-axis is visible as per the specification of the minimum boundary cell size parameter in the command file. The refinement in the center of the cube is due to the specification of the `minNumberOfCells` parameter in the command file. This refinement is constrained to a `"testbox"` window.

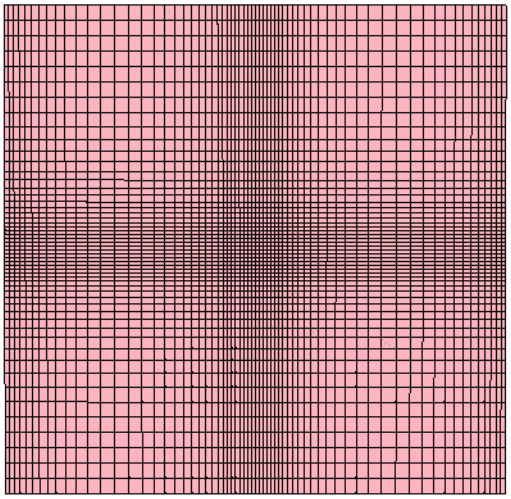


Figure 19 Smooth variation of cell size from minimum to maximum cell size according to specified grading factor

Using Boundary and Command Files to Generate Doping and Refinement

This example shows how to use the tensor-product mesh generator to represent an approximation of the actual regions defined in a boundary file. The geometry is shown in Figure 20. In this case, the default mesh generation parameters are used. A doping refinement section is provided in the command file.

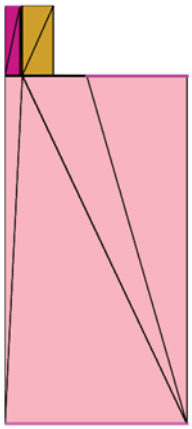


Figure 20 Geometry of an input file

Figure 21 shows the tensor mesh and the corresponding doping data. Note that the axis-aligned interfaces are represented accurately by the tensor mesh. However, if the geometry has a curved region, the resulting mesh will be an approximation of the boundary, as shown in Figure 22 on page 94.

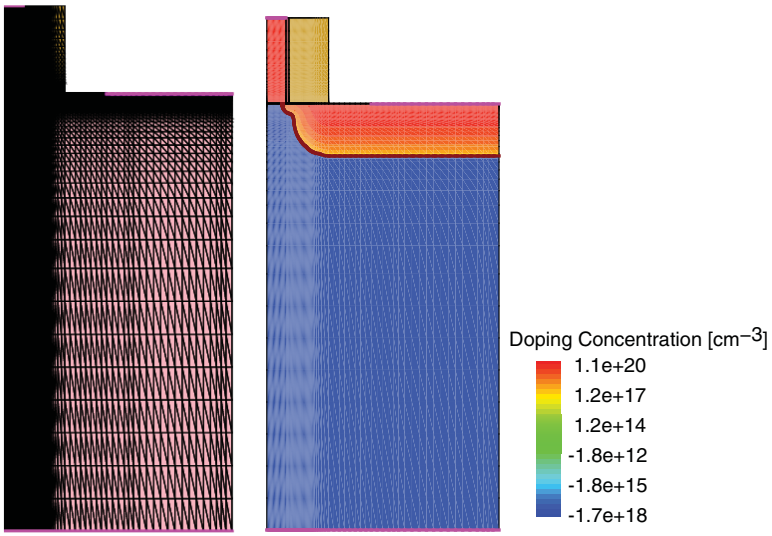


Figure 21 (*Left*) Tensor mesh and (*right*) the doping data interpolated onto tensor mesh

Figure 22 (*Left*) Actual curve region in the geometry and (*right*) corresponding approximation of this region in tensor mesh

Thin Regions

This example shows how insufficient cell resolution in a region will result in elements that are one dimension less than the model dimension. The geometry contains a thin aluminum region shown in Figure 23. Since the local cell size is not small enough to resolve this aluminum region, this region is represented as one-dimensional elements in the output as shown in Figure 24 on page 95.

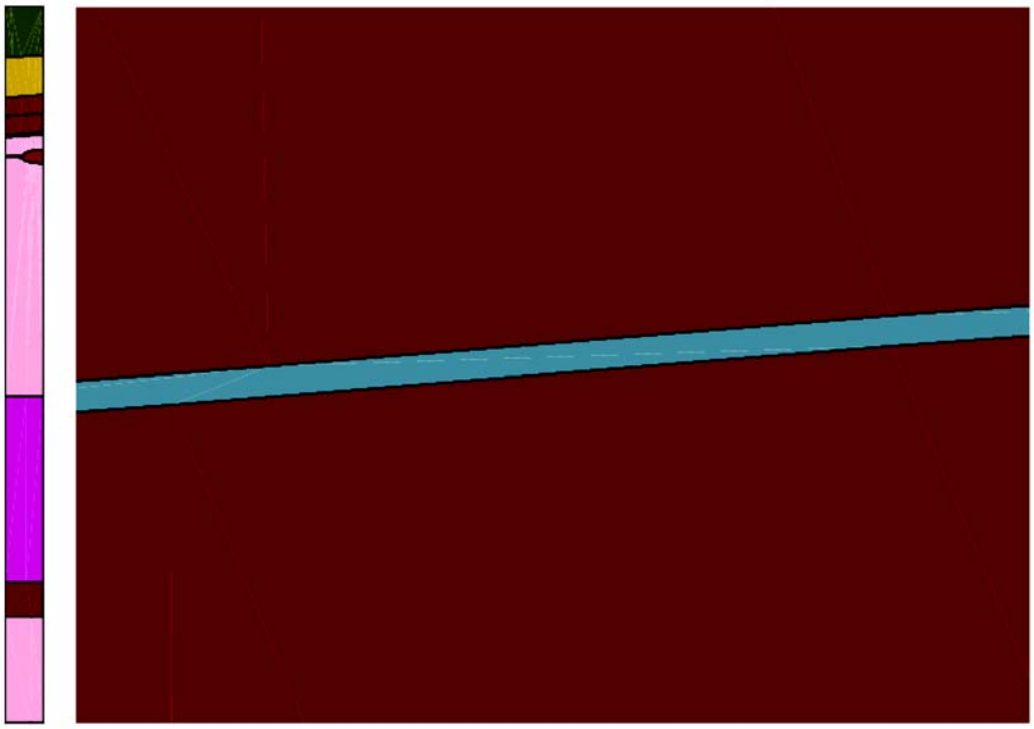


Figure 23 (*Left*) Geometry of the example and (*right*) detail of thin aluminum region

In Figure 24, the aluminum region is not resolved properly as the locally cell size is larger than the aluminum region. As a result, this region contains two faces and rest of the region is represented as a set of edges connecting the two faces. Similarly, in three-dimensional models, unresolved regions and contacts will be written as thin surface sheets. You will be given a warning indicating the presence of completely or partially unresolved regions.

The following is the command file used to generate the tensor-product mesh:

```
Tensor {
   Mesh {
      maxCellSize material "Oxide" 0.08
      maxCellSize material "Silicon" 0.08
      grading = { 1.1 1.1 1.1 }
   }
}
```

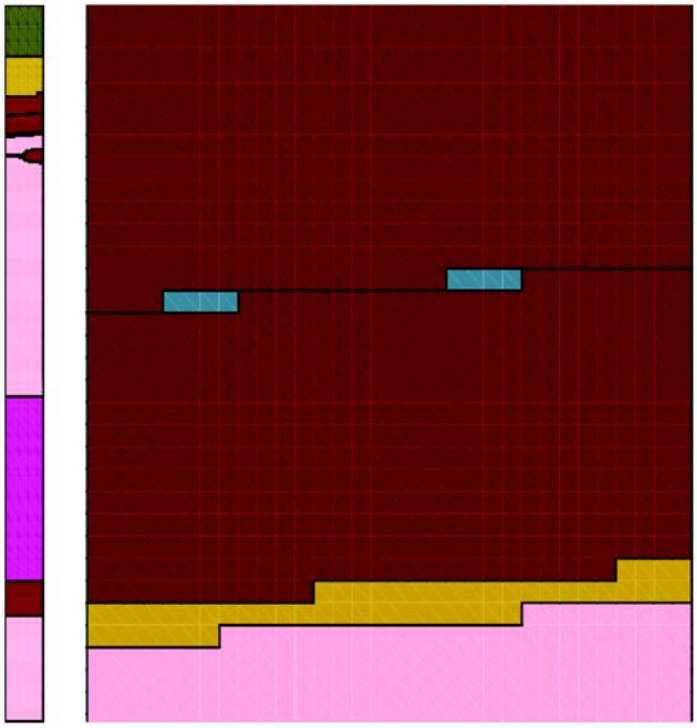


Figure 24 (*Left*) Corresponding tensor mesh and (*right*) detail of tensor mesh near aluminum region

Computing Cell Size Automatically (EMW Applications)

This example shows the command file structure that is used to compute cell sizes automatically using the tensor mesh generator. The tensor mesh generator reads the `Mesh` section of the command file first and then reads the `EMW` section. Since the cell size for the material `Insulator1` is defined in this section, it is not recomputed. The cell sizes for the rest of the materials are computed using the optical database table, which is defined in either the user-defined Sentaurus Device parameter file or the default Sentaurus Device parameter file.

The computed cell size is a function of the:

- Wavelength
- Nodes per wavelength
- Norm of a complex refractive index

In this example, the wavelength is equal to 2.0 µm and the nodes per wavelength is 5. The cell size is computed for all materials except `Insulator` since its cell size is specified in the `Mesh` section.

Among the materials present in the shown structure (see Figure 25), the computed cell size is smallest for `Aluminum`. Because of this, the mesh lines are more clustered in the corresponding region:

```
Tensor {
   Mesh {
      maxCellSize material "Insulator1" 0.1
   }
   EMW {
      wavelength = 2.0
      npw = 5
   }
}
```

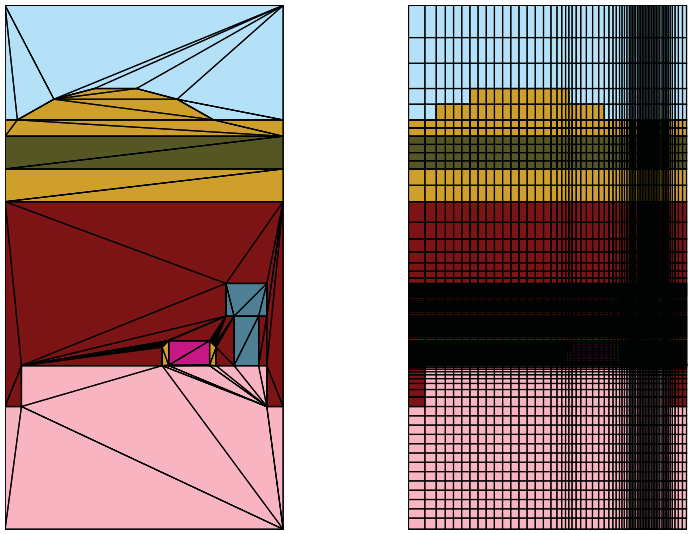


Figure 25 (*Left*) Boundary and (*right*) corresponding tensor mesh generated using the EnableEMW option in the IOControls section of the command file

CHAPTER 5 Tools Section

This chapter illustrates the use of the Tools section of the command file for Sentaurus Mesh.

Activating the Tools Section

To activate the `Tools` section in the command file of Sentaurus Mesh, specify either the `EnableSections` or the `EnableTools` option in the `IOControls` section of the command file (see IOControls Section on page 6).

Reflecting and Sweeping Mesh

In this example, a two-dimensional (2D) structure is taken and reflected. A three-dimensional (3D) mesh is then generated by sweeping the reflected mesh. The command file is:

```
Tools {
   Reflection {
      axis = xmin
      map "R.PolyReox" = "R.PolyReox_new"
   }
   Sweepmesh {
      extension = 0.1
      steps = 5
   }
}
```

The input mesh is shown in Figure 26 on page 98. The first step reflects the mesh structure about the `xmin` coordinate. The `map` statement renames the mirrored region `R.PolyReox` to `R.PolyReox_new`.

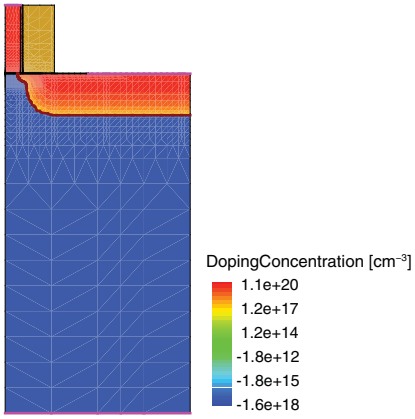


Figure 26 Input structure

The reflected mesh is shown in Figure 27. Since `Sweepmesh` is specified in the command file, the reflected mesh becomes input to this tool.

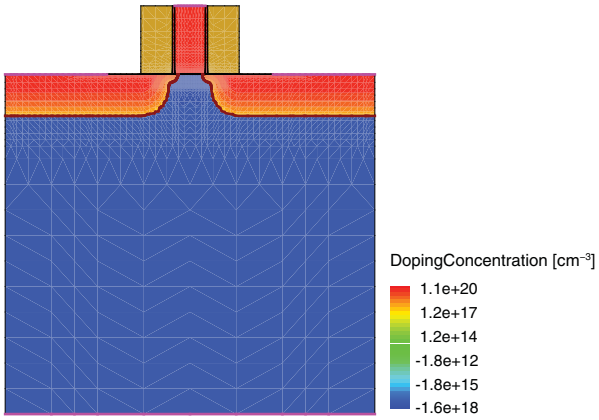


Figure 27 Reflected mesh

A 3D mesh is generated by sweeping the reflected mesh in the z-direction by $0.1\ \mu m$. Then, this mesh is divided into five sections along the z-direction as shown in Figure 28.

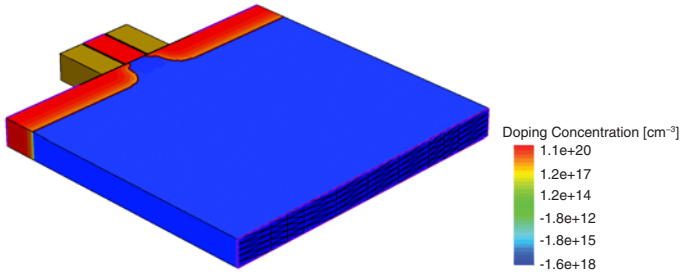


Figure 28 Mesh after being swept in the z-direction

Slicing a 3D Mesh Using a Plane and Its Location

In this example, a 3D mesh is sliced to obtain a 2D mesh. The command file is:

```
Tools {
   Slice {
      normal = (0 1 0)
      location = (0 0.0075 0)
   }
}
```

The input mesh is shown in Figure 29. The mesh is sliced with the y-plane placed at the specified location (`0 0.0075 0`). This results in a 2D mesh slice shown in Figure 30 on page 100.

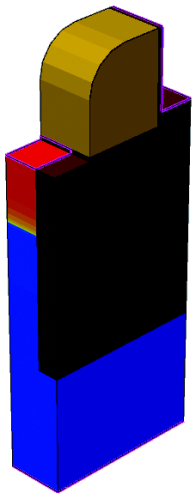


Figure 29 The input 3D mesh to be sliced

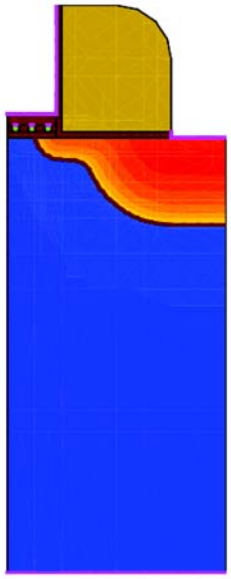


Figure 30 The 2D mesh slice generated from the mesh shown in Figure 29 on page 99

Cutting a 3D Mesh

In this example, a cube mesh is taken as an input and three cutting planes are used to create a wedge. The command file used in this example is:

```
Tools {
   Cut {
      normal = (0 0 1)
      location = (0.05 0.05 0.05)
   }
   Cut {
      normal = (0 -0.70711 0.70711)
      location = (0.05 0.05 0.05)
   }
   Cut {
      normal = (0 1 0)
      location = (0.05 0.05 0.05)
   }
}
```

In this code block, three cutting planes are specified. The input mesh is processed with the first cutting plane, and its output is given as an input to the next cutting plane. The input mesh and the final output mesh are shown in Figure 31.

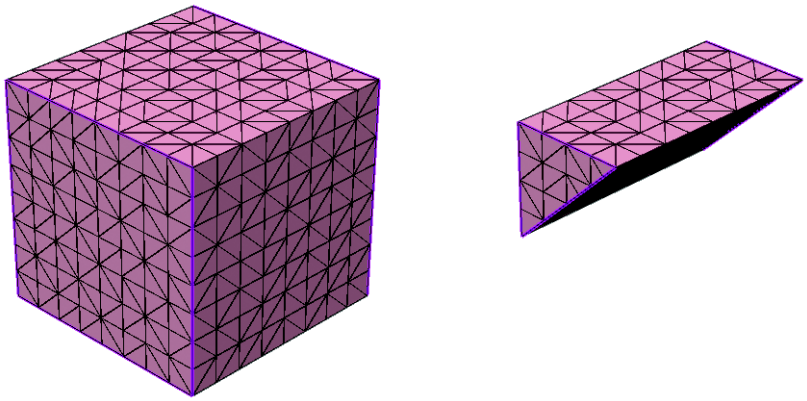


Figure 31 (*Left*) Input mesh and (*right*) final wedge created by using three cutting planes

Converting a Tetrahedral Mesh to a Hybrid Mesh

The following example translates a mesh and converts it to a hybrid mesh. The command file used in this example is:

```
Tools {
   Set Transformation {
      translation = ( 3 7 1 )
   }
   Apply Transformation
   Mesh2Hybrid
}
```

The log file contains information about a number of different element types in the converted mesh. In this example, approximately 55% of element reduction is achieved when compared to the input mesh.

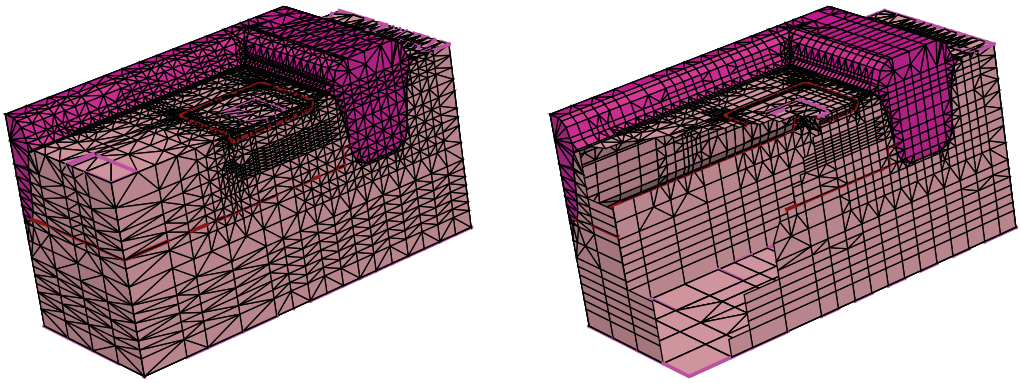


Figure 32 (*Left*) Tetrahedral mesh and (*right*) corresponding hybrid element produced by Mesh2Hybrid algorithm

Generating Randomized Doping From Continuous Doping

The following example illustrates a utility that randomizes a continuous doping. A mesh with continuous doping, along with a command file, is given as input. The command file for this example is:

```
Title "DopingRandomizer Example"
# Use "snmesh nmos00.cmd" to run. Assumes nmos00.tdr exists.

IOControls {
   EnableSections
}

Tools {
   RandomizeDoping {
      DopingAssignment = "Sano"
      # ContinuousContactDoping
      NumberOfRandomizedProfiles = 1
      FileIndex = 1
      Material "Silicon" {
         Species "BoronActiveConcentration" {
            ScreeningFactor = 2.5e6
            AutoScreeningFactor
         }
         Species "ArsenicActiveConcentration" {
            ScreeningFactor = 1.3e7
            AutoScreeningFactor
         }
      }
   }
}
```

The method chosen in this example is `"Sano"`. The number of randomized profiles is 1, and `FileIndex` is set to 1. Since only the material `"Silicon"` is specified, only silicon regions will be randomized. Other materials will retain their original continuous doping. Figure 33 shows the input structure mesh with continuous doping.

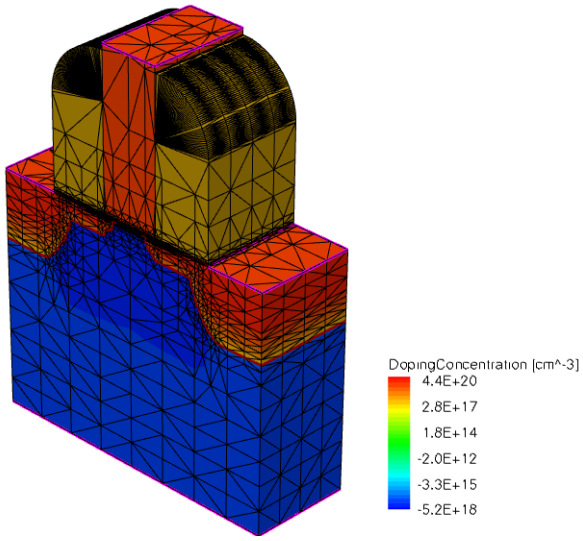


Figure 33 Input mesh with continuous doping

Figure 34 (*left*) shows the randomized doping generated using `DopingAssignment="Sano"`. Later, the command file is modified to use the other available methods. The middle structure in Figure 34 is generated using the NGP method, and third structure is generated using the CIC method.

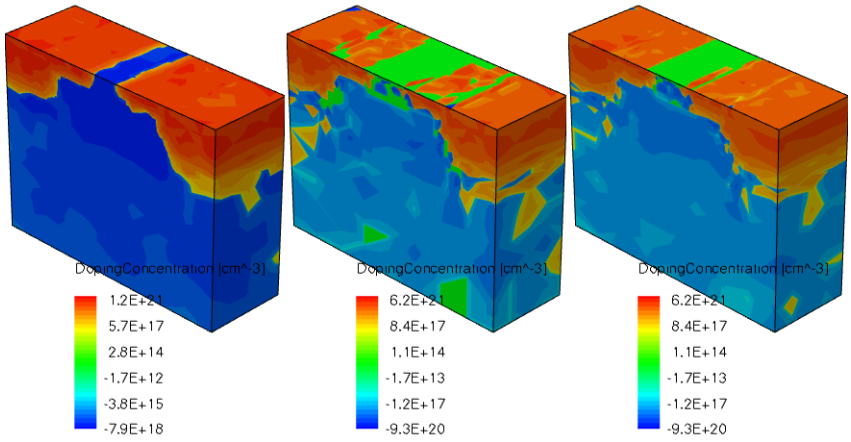


Figure 34 Meshes with randomized doping generated using the (*left*) Sano method, (*middle*) NGP method, and (*right*) CIC method

Slicing a 3D Mesh Using a Segment and a Direction

In this example, a 3D mesh is sliced to obtain a 2D mesh using a segment feature. The command file is:

```
Tools {
   Slice {
      Direction = Z
      Startpoint = (0.15 0.0)
      Endpoint = (0.15 0.75)
   }
}
```

In the above `Tools` section, a segment with a starting point and an endpoint on a constant Z-plane is specified. With this information, a bounding box of the input structure (shown in Figure 35 (*left*)) is computed and used in the construction of a plane defined by the bounding box coordinates of `[(0.15 0.0 zmin) (0.15 0.75 zmax)]`. The input boundary is sliced with this plane and the result is shown in Figure 35 (*right*). This boundary slice file also contains transformation information that can be used to place this slice back into 3D space for later applications.

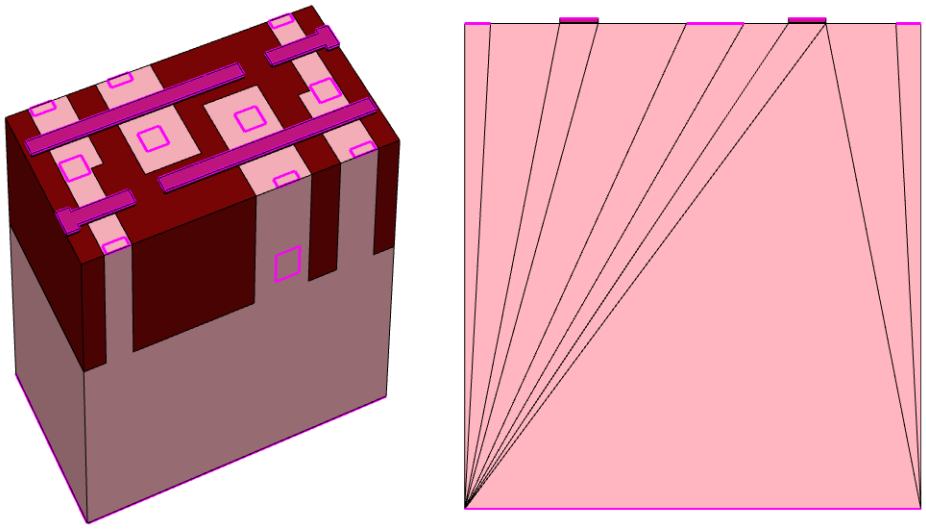


Figure 35 (*Left*) Input boundary and (*right*) 2D slice generated using slice utility

Creating Profiles in an Existing Mesh

This example shows the usage of the creating profiles utility. The command file contains information about an existing mesh and a mesh command file containing profile information. The profiles specified in the command file are created in the input mesh without changing the mesh itself. The command file for this example is:

```
Tools {
   CreateProfiles {
      SrcMesh = "n6_0_msh.tdr"
      CmdFile = "n6_msh.cmd"
   }
}
```

In the above `CreateProfiles` section, the source mesh file (shown in Figure 36 (*left*)) and the mesh command file are specified.

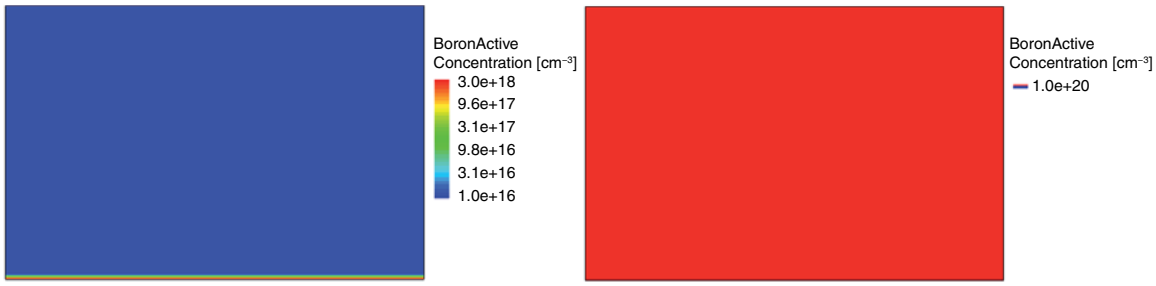


Figure 36 (*Left*) Input mesh showing BoronActiveConcentration profile before update and (*right*) mesh with updated BoronActiveConcentration

The mesh command file contains the following information related to `BoronActiveConcentration`:

```
Title "Untitled"

Definitions {
   Constant "substrateDop" {
      Species = "BoronActiveConcentration"
      Value = 1e+20
   }
}

Placements {
   Constant "substrateDop" {
      Reference = "substrateDop"
      EvaluateWindow { Element = region ["substrate"] }
   }
}
```

The `BoronActiveConcentration` profile in the input mesh is recreated without changing other profiles and, accordingly, the doping concentration is updated. The output mesh file is shown in Figure 36 on page 105 (*right*).

Stretching a Mesh

This example shows the usage of the stretch utility. The command file contains information about the location of the starting point of the stretch, the direction of the stretch, and the length of the stretch. The command file for this example is:

```
Tools {
   Stretch {
      location = (0.12 0.005 0)
      direction = X
      length = 0.05
   }
}
```

The input mesh is shown in Figure 37 (*left*). With the information in the command file, a new column of elements is added at the specified location. The output stretch mesh is shown in Figure 37 (*right*). After stretching, the length of the mesh in the specified direction is increased by a specified length. The unit of length is the same as the input mesh.

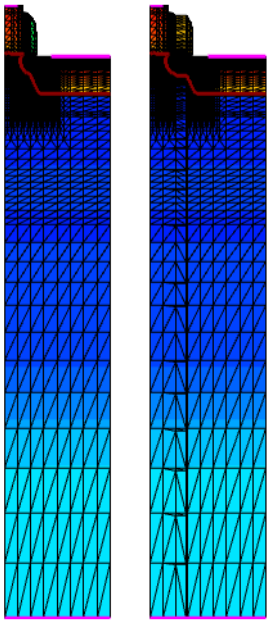


Figure 37 (*Left*) Input mesh before stretch and (*right*) mesh after stretch

CHAPTER 6 Delaunization Algorithm

This chapter describes the delaunization algorithm used by Sentaurus Mesh.

Overview

A delaunization algorithm is available for 3D models in Sentaurus Mesh. This algorithm is based on a conforming Delaunay triangulation–type of algorithm, but it is more stable, generating meshes for complex structures with sharp input angles that could not previously be handled. This delaunizer also produces fewer mesh nodes than the previous algorithm. Reference [1] is an excellent book on Delaunay mesh generation.

The algorithm uses two independent structures to generate the final mesh: a set of surface faces (for example, the input boundary and some isosurfaces, or rectangular faces originating from user-defined refinement inside Sentaurus Mesh) and a background three-dimensional generic Delaunay triangulation.

The algorithm works in the following way:

- Ridges and corners are classified.
- A set of protection spheres is generated around ridges and corners.
- A 2D surface delaunization algorithm is applied. This algorithm flips all nonridge edges that do not meet the Delaunay criterion.
- Each ridge that does not meet the Delaunay criterion is refined (see [2]).
- Each surface face that does not meet the Delaunay criterion is refined (see [2]).
- Each element that does not meet the quality criteria is refined.
- The surface faces that have not been recovered by refinement are recovered using a constrained Delaunay triangulation (CDT) algorithm (see [3][4]).
- Slivers are removed (see [5][6]).
- A material is assigned to each tetrahedron in the final triangulation.

Generating Ridges and Corners

During the first stage, the algorithm detects the faces that are coplanar. Every edge that bounds a coplanar set of faces is labeled a ridge. Every point that connects two non-collinear ridges is labeled a corner.

By default, two faces are coplanar if the angle between them is less than `coplanarityAngle` and the surface deformation that can result from flipping the common edge is less than `coplanarityDistance`.

Protecting Ridges and Corners

In general, conforming Delaunay algorithms do not perform well if the input contains sharp angles between adjacent faces on the surface (in general, of less than 60°). A generic algorithm would refine excessively around ridges and corners that define a very sharp angle. Occasionally, generic algorithms do not stop and the algorithms collapse.

The algorithm for ridge and corner refinement carefully refines around sharp corners and ridges, defining a set of spheres that protect these entities. Refinement points that are inside these spheres are snapped to the surface of the sphere. This produces constructions that resemble isosceles triangles, which are well suited to Delaunay-type algorithms because isosceles triangles contain their circumscribed centers inside them.

Conforming Delaunay Triangulation Algorithm

The conforming Delaunay triangulation (CDT) algorithm enables the delaunizer to produce meshes that are near-Delaunay after relaxing the Delaunay criterion.

After the faces have been refined to meet the (possibly relaxed) Delaunay criterion, some surface faces may be missing from the background 3D Delaunay mesh. The CDT algorithm inserts those faces into the background triangulation using a sequence of 3D face flips.

This algorithm is very complex, therefore, you can expect long runtimes if the Delaunay criterion is relaxed too much at locations with many faces to be recovered (such as locations with a lot of refinement in Sentaurus Mesh).

Optimizing Elements

After the CDT algorithm is finished, the quality of the elements in the mesh may not be optimal. Therefore, the algorithm performs an extra refinement step, which eliminates all elements that do not meet the quality criteria specified by users. Two quality criteria are available:

- The maximum solid angle inside an element.
- The maximum ratio between the circumscribed spheres of neighboring elements.

Any element that does not meet the quality criteria will be refined. The algorithm used to refine the elements is based on the Delaunay refinement technique, which inserts a node at the Voronoï center of the element and updates the neighboring triangulation. If the Voronoï center of the element lies too close to the surface, the surface will be refined.

Eliminating Slivers

The last step in the delaunization involves the elimination of sliver elements. To perform this, the algorithm uses a variation of the sliver exudation technique. This technique assigns weights to the nodes in the triangulation and uses them to compute a weighted Delaunay triangulation. The weights are increased selectively to eliminate slivers locally in the triangulation.

The sliver elimination step changes the regular Voronoï diagram, producing Voronoï cells that have negative sides.

The amount of damage is proportional to the weight applied to the mesh nodes. Therefore, the algorithm includes a parameter, called `sliverDistance`, to control the amount of damage to the mesh. This parameter represents the maximum weight applied to a mesh node.

References

[1] S.-W. Cheng, T. K. Dey, and J. R. Shewchuk, *Delaunay Mesh Generation*, Boca Raton, Florida: CRC Press, 2013.

[2] J. R. Shewchuk, “Mesh Generation for Domains with Small Angles,” in *16th Annual Symposium on Computational Geometry*, Hong Kong, pp. 1–10, June 2000.

[3] J. R. Shewchuk, “Constrained Delaunay Tetrahedralizations and Provably Good Boundary Recovery,” in *Proceedings of the 11th International Meshing Roundtable*, Ithaca, NY, USA, pp. 193–204, September 2002.

[4] J. R. Shewchuk, "Updating and Constructing Constrained Delaunay and Constrained Regular Triangulations by Flips," in *19th Annual Symposium on Computational Geometry*, San Diego, CA, USA, pp. 181–190, June 2003.

[5] S.-W. Cheng *et al*., "Sliver Exudation," *Journal of the ACM*, vol. 47, no. 5, pp. 883–904, 2000.

[6] H. Edelsbrunner and D. Guoy, "An Experimental Study of Sliver Exudation," in *Proceedings of the 10th International Meshing Roundtable*, Newport Beach, CA, USA, pp. 307–316, 2001.

APPENDIX A Formulas for Analytic Profiles

Sentaurus Mesh implements a complete set of analytic models to describe a wide range of different situations. The reason for implementing analytic profiles is to have a flexible tool to substitute process simulation results efficiently and within a reasonable time.

This appendix discusses:

- General concepts.
- The models that are available along the primary direction.
- The models that are available along the lateral direction.

Although the formulas are designed according to the models associated with impurity concentrations, the analytic profiles can be used for any type of variable defined in the output files.

General Concepts

The impurity concentrations can be represented by a set of 1D, 2D, and 3D analytic models. To describe each analytic model, two main directions must be defined: the *primary direction* that is perpendicular to the reference region and the *lateral direction* that is parallel to the reference region.

Along each direction, one function is defined, that is, the *primary function* and *lateral function*. The correct combination of both functions allows you to have an analytic description of a species concentration.

Local Coordinate Systems, Valid Domains, and Reference Regions

The valid domain for the analytic models depends on the reference region, which is defined using a dimension-dependent geometric element, and it is placed along the lateral direction. By combining the reference region and primary direction, it is possible to define a local coordinate system for each analytic function.

One-Dimensional Profiles

One-dimensional profiles require only the definition of the primary function, which is applied along the x-axis. The primary direction and valid domain are defined using a vector. The reference region for a profile is defined by using a geometric element, that is, a point. Figure 38 shows the scheme used for the 1D case.

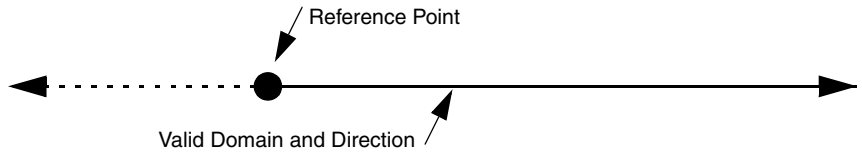


Figure 38 Primary direction in 1D

Two-Dimensional Profiles

For 2D profiles, the reference region is defined using a *baseline*. The primary direction is the normal vector to the baseline and the lateral direction is parallel to the baseline. Figure 39 shows the general scheme of the local coordinate system and the valid domain. The valid domain for both the primary and lateral functions is defined by sweeping the primary direction vector along the lateral direction.

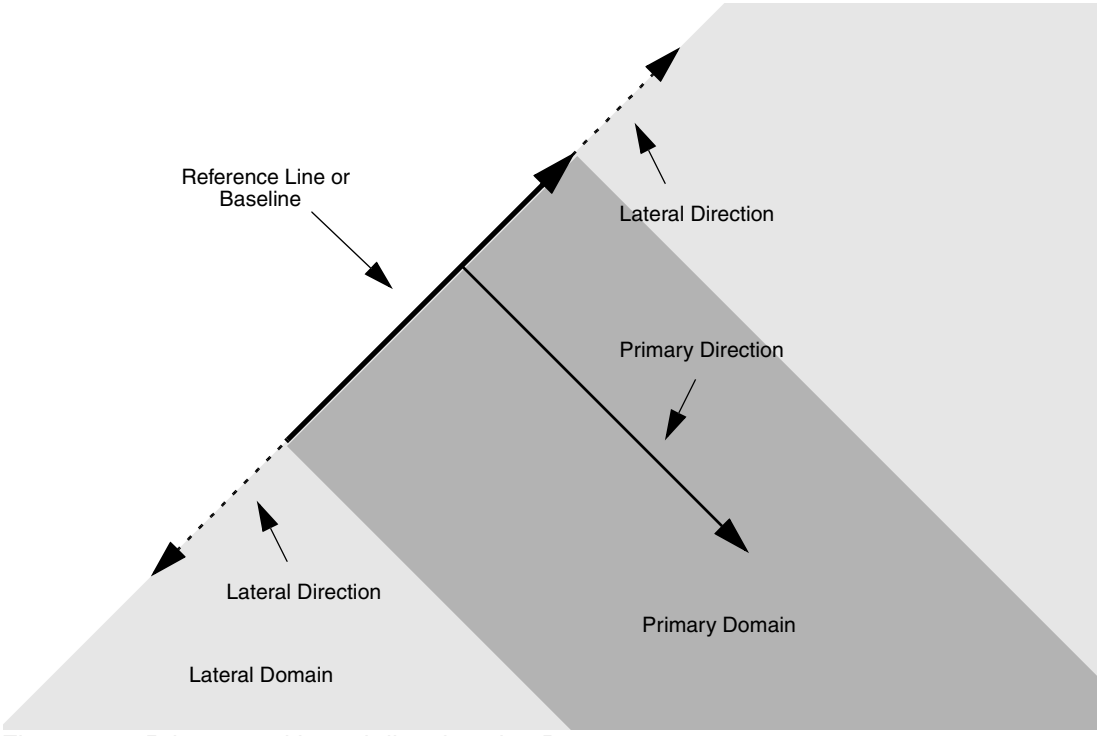


Figure 39 Primary and lateral directions in 2D

Three-Dimensional Profiles

For 3D profiles, the reference region is defined using a *surface*. The primary direction is the normal vector to the surface and the lateral direction is the plane perpendicular to the primary direction. Figure 40 shows the general scheme of the local coordinate system and the valid domain. The valid domain for both primary and lateral functions is defined by sweeping the primary direction vector along the surface.

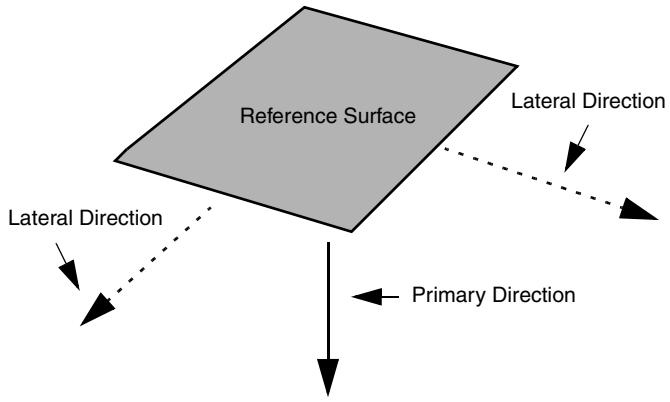


Figure 40 Primary and lateral directions in 3D

General Implantation Models

In general, impurity concentrations can be expressed as:

$$\text{doping}(\vec{x}_p, \vec{x}_l) = g\langle \vec{x}_p \rangle \cdot f\langle \vec{x}_l \rangle \quad (3)$$

where:

- $g\langle \vec{x}_p \rangle$ represents the primary function in the local coordinate system.
- $f\langle \vec{x}_l \rangle$ represents the lateral function in the local coordinate system.

The most important functions used as models are Gaussian functions and error functions. For the remainder of this appendix, functions along the primary direction are referred to as $g\langle y \rangle$ and functions along the lateral direction, as $f\langle x \rangle$. The indices y and x are important to distinguish parameters among the different directions.

Each model is defined by the minimum set of parameters. This section presents a basic formulation of each model by using the minimum set of parameters. Subsequent sections show how to obtain this minimum set from different input or initial conditions.

Gaussian Function

The minimum set of parameters to define a Gaussian function is:

- Peak concentration (C_{peak}) [cm^{-3}]
- Peak position (y_{peak}) [µm]
- Length (GLength_y) [µm] or standard deviation (stdDev_y) [µm]

Using these parameters, the Gaussian is defined by:

$$g(y) = C_{\text{peak}} \cdot \exp\left(-\frac{1}{2} \cdot \left[\frac{y - y_{\text{peak}}}{\text{stdDev}_y}\right]^2\right) = C_{\text{peak}} \cdot \exp\left(-\left[\frac{y - y_{\text{peak}}}{\text{GLength}_y}\right]^2\right) \quad (4)$$

Figure 41 shows the model schematically.

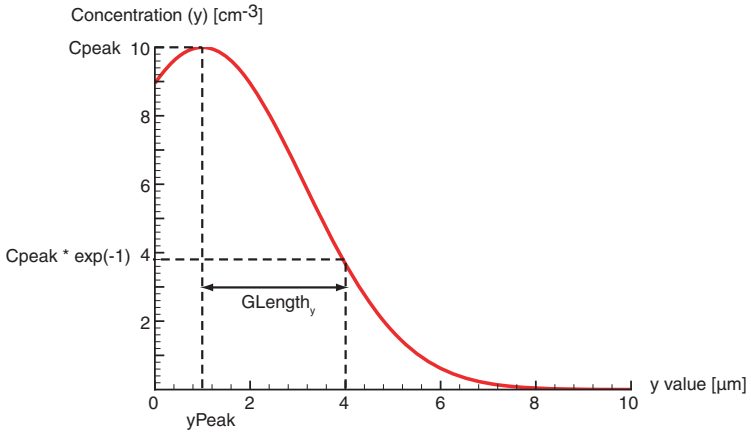


Figure 41 General shape of Gaussian functions

Error Function

The minimum set of parameters to define an error function as a doping profile is:

- Maximum concentration (C_{max}) [cm^{-3}]
- Symmetry position (y_{sym}) [µm]
- Length (ELength_y) [µm]

Using these parameters, the error function is defined by:

$$g(y) = \frac{C_{\text{max}}}{2} \cdot \left(1 + erf\left[\frac{y_{\text{sym}} - y}{\text{ELength}_y}\right]\right) = \frac{C_{\text{max}}}{2} \cdot \left(1 - erf\left[\frac{y - y_{\text{sym}}}{\text{ELength}_y}\right]\right) \quad (5)$$

The function is symmetric with respect to the inflection point. Figure 42 shows the feature.

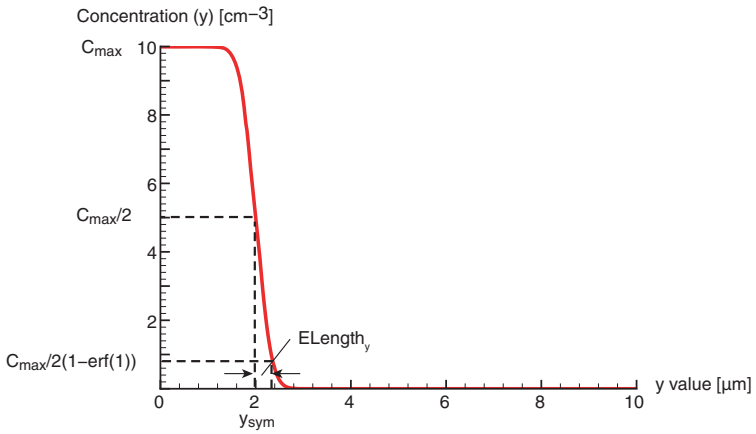


Figure 42 General shape of error functions

Other Relevant Parameters

To have flexible models, some special parameters must be considered. These are not included in the standard formulation. However, by applying some definitions, the basic set can be obtained from them.

Dose

From a process simulation perspective, implantation functions are determined giving the dose concentration of the profiles. The peak concentration value can be obtained from the *Dose* (see Available Models Along the Primary Direction on page 116). Dose is given in atoms per cm^{-2}.

The general definition of Dose is:

$$\text{Dose} = \int_0^\infty g(y)dy \tag{6}$$

For Gaussian functions, the Dose is represented as:

$$\text{Dose} = \int_0^\infty C_{\text{peak}} \cdot \exp\left(-\frac{1}{2} \cdot \left[\frac{y - y_{\text{peak}}}{\text{stdDev}_y}\right]^2\right) dy \tag{7}$$

$$\text{Dose} = \frac{C_{\text{peak}} \cdot \sqrt{\pi} \cdot \text{stdDev}_y}{\sqrt{2}} \cdot \left(1 + erf\left[\frac{y_{\text{peak}}}{\sqrt{2} \cdot \text{stdDev}_y}\right]\right) \tag{8}$$

For error functions, the Dose is defined as:

$$\text{Dose} = \int_0^{\infty} \frac{C_{\max}}{2} \cdot \left(1 + erf\left[\frac{y_{\text{sym}} - y}{\text{ELength}_y}\right]\right) dy \tag{9}$$

$$\text{Dose} = \frac{C_{\max} \cdot \text{ELength}_y}{2} \cdot \left(\frac{y_{\text{sym}}}{\text{ELength}_y} \cdot \left[1 + erf\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)\right] + \frac{1}{\sqrt{\pi}} \cdot \exp\left[-\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)^2\right]\right) \tag{10}$$

Values at the Junction

Junction Concentration and *Depth* are parameters used to define either Gaussian or error functions. A complete description of these parameters and how they can replace the standard deviation in the basic formulation is explained in Available Models Along the Primary Direction.

Length

For Gaussian functions, GLength represents the distance between the peak position and a place where the concentration decays by a factor of exp(–1) (36%) with respect to the peak concentration (see Figure 41 on page 114). The relationship between the length and standard deviation for Gaussian functions is:

$$\text{GLength}_y = \sqrt{2} \cdot \text{stdDev}_y \tag{11}$$

Available Models Along the Primary Direction

The following models in Sentaurus Mesh are applied along the primary direction:

- Gaussian functions
- Error functions
- Constant functions
- 1D external profiles

Gaussian Functions

The basic set for Gaussian functions is formed by C_{peak}, y_{peak}, and stdDev_y. According to user input, the basic set of parameters can be specified in six different ways depending on the parameters used to calculate C_{peak} and stdDev_y:

- Peak Concentration and Standard Deviation

  The basic set is complete (see Eq. 4) and no basic parameters are computed.

- Peak Concentration and Length

  Standard Deviation is computed from GLength using:

$$\text{stdDev}_y = \frac{\text{GLength}_y}{\sqrt{2}} \tag{12}$$

- Dose and Standard Deviation

  Given Dose and Standard Deviation, the Peak Concentration value is calculated using:

$$C_{\text{peak}} = \frac{\text{Dose} \cdot \text{factor} \cdot \sqrt{2}}{\sqrt{\pi} \cdot \text{stdDev}_y \cdot \left(1 + erf\left[\frac{y_{\text{peak}}}{\sqrt{2} \cdot \text{stdDev}_y}\right]\right)} \tag{13}$$

  where $\text{factor} = 10^4$ because Dose is in cm^{-2}.

- Dose and Length

  Given Dose and GLength, the Standard Deviation is computed from Eq. 12, and the Peak Concentration is computed from Eq. 13.

- Peak Concentration and values at the junction

  Standard Deviation is computed from the values at the junction using:

$$\text{stdDev}_y = \frac{y_{\text{depth}} - y_{\text{peak}}}{\sqrt{-2 \cdot \ln(C_{\text{atDepth}} / C_{\text{peak}})}} \tag{14}$$

  NOTE C_{peak} must be greater than C_{atDepth}.

- Dose and values at the junction

  First, Standard Deviation is computed from:

$$\frac{C_{\text{atDepth}} \cdot \sqrt{\pi} \cdot \text{stdDev}_y \cdot \left(1 + erf\left[\frac{y_{\text{peak}}}{\sqrt{2} \cdot \text{stdDev}_y}\right]\right)}{\sqrt{2} \cdot \text{Dose} \cdot \text{factor}} = \exp\left(-\frac{1}{2} \cdot \left[\frac{y_{\text{depth}} - y_{\text{peak}}}{\text{stdDev}_y}\right]^2\right) \tag{15}$$

Second, using stdDev_y, Peak Concentration is computed as in C.

NOTE Eq. 15 is an implicit equation and Dose is in cm^{-2}.

Error Functions

For error functions, the basic set of parameters includes $C_{\max}$, y_{sym}, and ELength_y and can be computed in four ways:

- Maximum Concentration and Length

  The basic set is complete and no parameters are computed (see Eq. 5).

- Dose and Length

  Maximum Concentration is computed from Dose using:

$$C_{\max} = \frac{2 \cdot \text{Dose}}{\text{ELength}_y} \cdot \text{factor} \cdot \left(\frac{y_{\text{sym}}}{\text{ELength}_y} \cdot \left[1 + erf\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)\right] + \frac{1}{\sqrt{\pi}} \cdot \exp\left[-\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)^2\right]\right)^{-1} \quad (16)$$

  where $\text{factor} = 10^4$ because Dose is in cm^{-2}.

- Maximum Concentration and values at the junction

  ELength can be computed from:

$$erf\left(\frac{y_{\text{sym}} - y_{\text{depth}}}{\text{ELength}_y}\right) = \frac{2 \cdot C_{\text{atDepth}}}{C_{\max}} - 1 \quad (17)$$

  NOTE Eq. 17 is an implicit equation.

- Dose and values at the junction

  Maximum Concentration and ELength are computed using the following implicit equations, which follow from Eq. 16 and:

$$\text{Dose} \cdot \text{factor} \cdot \left(1 + erf\left[\frac{y_{\text{sym}} - y_{\text{depth}}}{\text{ELength}_y}\right]\right) = C_{\text{atDepth}} \cdot \text{ELength}_y \cdot \left(\frac{y_{\text{sym}}}{\text{ELength}_y} \cdot \left[1 + erf\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)\right] + \frac{1}{\sqrt{\pi}} \cdot \exp\left(-\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)^2\right)\right) \quad (18)$$

$$C_{\max} = \frac{2 \cdot \text{Dose}}{\text{ELength}_y} \cdot \text{factor} \cdot \left(\frac{y_{\text{sym}}}{\text{ELength}_y} \cdot \left[1 + erf\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)\right] + \frac{1}{\sqrt{\pi}} \cdot \exp\left[-\left(\frac{y_{\text{sym}}}{\text{ELength}_y}\right)^2\right]\right)^{-1} \quad (19)$$

Constant Functions

Constant functions are useful to define substrate doping mathematically:

$$g(y) = \text{Constant} \tag{20}$$

1D External Profiles

Real 1D process simulation results can be read along the primary direction. To complete the 2D profile and 3D profile, an analytic lateral function is added.

The values that do not appear in the file are interpolated using an interpolation function. Every species has a corresponding interpolation function predefined in the `datexcodes.txt` file. These functions can be linear, arsinh, or logarithmic.

If h is an interpolation function, the value at point y is computed from an external 1D profile as follows:

$$g(y) = \begin{cases} \text{data}_i & y = y_i \\ h^{-1}\left(\frac{y - y_i}{y_{i+1} - y_i} \cdot h(\text{data}_{i+1}) + \frac{y - y_{i+1}}{y_{i+1} - y_i} \cdot h(\text{data}_i)\right) & y_i < y < y_{i+1} \end{cases} \tag{21}$$

Lateral or Decay Functions

The lateral or decay functions are evaluated on the valid lateral domain (see Figure 39 on page 112 and Figure 40 on page 113). They are defined as the decay along the lateral direction and depend on the distance from the valid primary domain of the point to evaluate. For 2D, this distance is calculated using the baseline as reference. For 3D, the distance is computed using the *surface* as reference. The three available models to apply are:

- Gaussian function
- Error function
- No function

NOTE Lateral or decay functions are not valid for one dimension.

Lateral Gaussian Function

The equation applied is:

$$f(x) = \exp\left(-\frac{1}{2} \cdot \left[\frac{x_{\text{closest}P} - x}{\text{stdDev}_x}\right]^2\right) \tag{22}$$

According to Eq. 22, the required value from the user is the standard deviation, stdDev_x, along the lateral direction. There are three ways to define it:

- Provide the value explicitly.
- Provide a factor with respect to the standard deviation along the primary direction:

$$\text{stdDev}_x = \text{Factor}_x \cdot \text{stdDev}_y \tag{23}$$

- Give the length of the Gaussian function:

$$\text{GLength}_x = \text{stdDev}_x \cdot \sqrt{2} \tag{24}$$

By using this function, the decay begins outside the primary domain, that is, the overlap between the primary, lateral, and decay domains is zero. Figure 43 shows this effect.

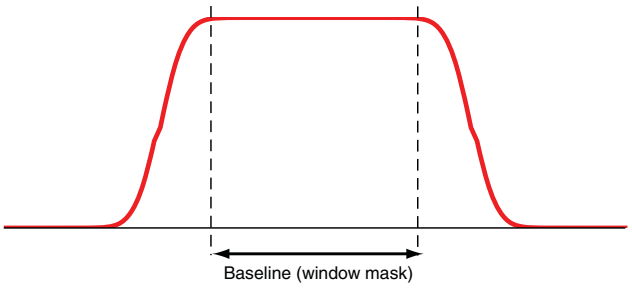


Figure 43 Using Gaussian function as lateral function in two dimensions

Lateral Error Function

By default, when specifying an error function as a lateral function in an analytic profile, the following equation is applied:

$$f(x) = \frac{1}{2} \cdot \left(1 + erf\left[\frac{x_{\text{closest}P} - x}{\text{ELength}_x}\right]\right) \tag{25}$$

According to Eq. 25, the required value from the user is the length for the error function, ELength_x, along the lateral direction.

There are two ways to define it:

- Provide the value explicitly.
- Provide a factor with respect to the length along the primary direction:

$$\mathrm{ELength}_x = \mathrm{Factor}_x \cdot \mathrm{ELength}_y \tag{26}$$

For this model, the overlap of the primary, lateral, and decay domains is not zero. The lateral decay starts inside the primary domain as shown in Figure 44.

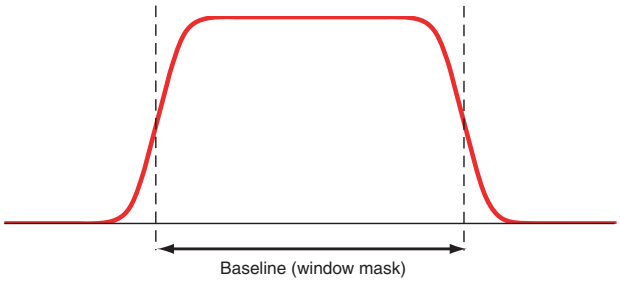


Figure 44 Using error function as lateral function in two dimensions

In some situations, the previous formulation can lead to a change in the total dose defined by the analytic profile. In those cases, you can use the `lateralDiffusion` parameter in the `Interpolate` section of the Sentaurus Mesh command file to change the formula used to calculate the error function (see Interpolate Section on page 29):

$$f(x) = \frac{1}{2} \cdot \left(erfc\left[\frac{x - x_{\max}}{\mathrm{ELength}_x}\right] - erfc\left[\frac{x - x_{\min}}{\mathrm{ELength}_x}\right] \right) \tag{27}$$

For higher dimensions:

$$f(x, y, z) = f(x) \cdot f(y) \cdot f(z) \tag{28}$$

These formulas are used only if the reference element is rectangular. In this case, $x_{\min}$ and $x_{\max}$ are the minimum and the maximum coordinates of the reference element, respectively.

No Lateral Function

This property is valid when Factor is equal to zero. In this case, the value of the lateral function is given by:

$$f(x) = \begin{cases} 1 & x \in \mathrm{PrimaryDomain} \\ 0 & x \notin \mathrm{PrimaryDomain} \end{cases} \tag{29}$$

The lateral domain is null.

APPENDIX B Doping Function for Discrete Dopants

This appendix describes the doping function that is used to transform discrete dopants into a continuous doping profile.

Sentaurus Mesh can be used to create continuous doping profiles from discrete dopant distributions obtained from Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC). This is accomplished by associating a doping function with each discrete dopant. The union of all such doping functions defines the final doping profile for the structure.

Doping Function

It has been suggested [1] that the charge density associated with a discrete dopant be can separated into short-range and long-range portions, and that the long-range portion is appropriate for inclusion in drift-diffusion device simulators. Sentaurus Mesh uses the long-range portion of the number density associated with a discrete dopant suggested in [1]:

$$n(r) = N_f \cdot \frac{k_c^3}{2\pi^2} \frac{\sin(k_c r) - (k_c r)\cos(k_c r)}{(k_c r)^3} \tag{30}$$

In this expression, r is the distance from the discrete dopant, k_c is the inverse of the screening length, and N_f is a normalization factor such that the integral of $n(r)$ over the entire simulation space becomes unity. Note that the above function is oscillatory and becomes negative for certain values of $k_c r$ (see Figure 45 on page 124). In Sentaurus Mesh, however, the above function is cut off at the first zero of $n(r)$. That is:

$$\begin{aligned} n(r) &= N_f \cdot \frac{k_c^3}{2\pi^2} \frac{\sin(k_c r) - (k_c r)\cos(k_c r)}{(k_c r)^3} \quad , \quad k_c r < 4.4934 \\ &= 0 \quad , \quad k_c r \geq 4.4934 \end{aligned} \tag{31}$$

In this case, the normalization factor is taken to be $N_f = 0.59688$.

NOTE This normalization factor assumes that the function given in Eq. 31 does not extend outside the simulation space. In general, this will not be true for discrete dopants located near boundaries.

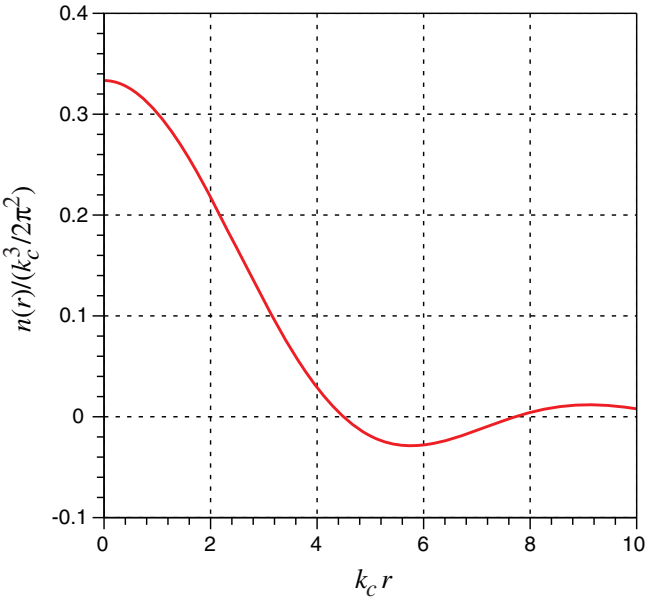


Figure 45 Long-range number density associated with a discrete dopant

Cut-off Parameter

The inverse of the cut-off parameter, $1/k_c$, is the screening length. Different charge screening models suggest different expressions for k_c as a function of impurity concentration. One model suggests that k_c is the inverse of the Debye length:

$$k_c = \sqrt{\frac{Ne^2}{\varepsilon_{\mathrm{Si}} k_B T}} \tag{32}$$

where N is the impurity concentration, e is the electronic charge, $\varepsilon_{\mathrm{Si}}$ is the permittivity of silicon, k_B is the Boltzmann constant, and T is temperature. However, the paper [1] prefers a charge screening model that gives k_c simply as:

$$k_c \approx 2N^{1/3} \tag{33}$$

In practice, k_c can be used as a fitting parameter, for example, by comparing the threshold voltage for a large MOSFET when the present doping model is used with the threshold voltage obtained with a standard continuum doping model.

In Sentaurus Mesh, k_c is a user-adjustable parameter and is called the `ScreeningFactor`. It is part of the `Particle` definition and it can be specified separately for each `Species`.

References

[1] N. Sano *et al*., "On discrete random dopant modeling in drift-diffusion simulations: physical meaning of 'atomistic' dopants," *Microelectronics Reliability*, vol. 42, no. 2, pp. 189–199, 2002.