Structure Generator and Mesher

Informative session

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Overview

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- Onfiguring structure generator
- Optimize Python interface
- 4 Editing RefWins
- G Analytical doping profiles
- 6 Importing GDS layouts
- Ø Graphical user interface
- 8 Conclusion
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The structure generator reads in the size and shape of the device from the *config* file. Salient features of the structure generator are –

- Creates a 2D or 3D device composed of many (possibly intersecting) regions of shapes -
 - Axis-aligned rectangle or cuboid,
 - 2D Polygon or 3D polyhedron from vertices,
 - Special shapes 2D: ellipse 3D: ellipsoid, cylinder, cone.
- Performs the required shape modifications
 - 2D or 3D Boolean operations add, clip, subtract shapes
 - 2D or 3D Shape transformations translate, rotate, scale, mirror shapes
 - 2D or 3D Shape rounding, chamfering, offsetting, stretching
 - 2D Shape sweep to create prisms, pyramids, pipes, revolutions
- Doping definitions of analytic profiles such as Gaussian, exponential, linear, or user-defined can be set.
- Specifies mesh refinements globally or regions-wise or in specific areas.
- Python interface enables convenient scripting and integration.
- Import *GDS* layout file to create masks for doping, etching, or deposition.

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The mesher tool creates the specified type of mesh using the mesh refinements set by the user in the config file. Following mesh are supported.

- FEM-mesh: A triangular (2D devices) or tetrahedral (3D devices) finite-elements based mesh. It is used for electrical drift-diffusion transport simulations, and for dopant diffusion process simulations.
- Tensor-mesh: A rectangular (2D devices) or cubic (3D devices) grid based mesh. It is used for optical FDTD simulations, BPM simulations. It is also used for electrical QT simulations with NEGF formalism.
- Triangle¹ mesh: External 2D mesher,
- TQMesh²mesh: External 2D mesher,
- TetGen³mesh: External 3D mesher,
- *CGAL*⁴mesh: External 3D mesher.

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¹Jonathan Richard Shewchuk, *Triangle: Engineering a 2D Quality Mesh Generator and Delaunay Triangulator*. Lecture Notes in Computer Science, pages 203-222, Springer-Verlag, Berlin, May 1996

²Jonathan Richard Shewchuk, *TQMesh*

³Si, Hang (2015): *TetGen, a Delaunay-Based Quality Tetrahedral Mesh Generator*, ACM Transactions on Mathematical Software 41, S. 1–36.

⁴P. Alliez, et al: CGAL User and Reference Manual, CGAL Editorial Board, 5.6.1

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Config file for structure generation

```
Device:
  Name = "Diode":
 MeshType = "FEM";
  Simulation = "DD";
RefWin*RefSi: {
  Position: ([-1.0, -0.2, 0.], [1., 0.2, 0.]);
  Shape = "Rectangle":
RefWin*RefCathode: {
  Position: ([0.999, -0.25, 0.], [1.001, 0.25, 0.]);
  Shape = "Rectangle";
RefWin*RefPDoping:
  Position: ([-1.001, -0.25, 0.], [0., 0.25, 0.]);
  Shape = "Rectangle";
RefWin*RefNDoping:
  Position: ([0.0, -0.25, 0.], [1.001, 0.25, 0.]);
  Shape = "Rectangle":
Region*RegSi:
  RefWin = ["RefSi"]:
  Material = "Silicon":
  //MaxEdgeLength = 0.05;
```





- Device: selects the mesh-type and intent of simulation.
- RefWin: Shapes which can be used for a variety of purposes, by linking them to Region, Contact, Doping, etc.
- Region: Set RefWin list and the Material.
- Material: New material defined by adding a Material.cfg file in the working directory.

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Config file for structure generation

```
MeshDef*MDefSiTop: {
  RefWin = "RefAll":
  X: {cen = 0., minspacing = 0.0001,
      maxspacing = 0.05, incr = 1.3 }
  Y: {cen = 0., minspacing = 0.025,
      maxspacing = 0.025, incr = 1.
DopingDef*Pdoping:
  RefWin = "RefPDoping";
  Type = "Constant":
  Concentration = 5E16:
  Dopant = "Boron":
. . .
Contact*Cathode: {
  RefWin = ["RefCathode"]
Contact * Anode · (
  RefWin = ["RefAnode"]
```

- MeshDef: Meshing definition followed in the specified RefWin.
 - cen: center of the refined mesh.
 - minspacing: minimum spacing at the cen.
 - maxspacing: maximum spacing in the RefWin.
 - incr: rate of increment of mesh spacing.





- DopingDef: Doping of the vertices in the RefWin.
- Contact: Vertices in the specified RefWin are set as contact vertices.

2D Mesh Types

Set the mesh-type in Device as follows -

```
Device: {
   MeshType = "FEM"; // "Tensor" or "TetMesh"
}
```

Internal mesh engines -

- FEM-mesh: A triangular (2D devices) or tetrahedral (3D devices) finite-elements based mesh.
- Tensor-mesh: A rectangular (2D devices) or cubic (3D devices) grid based mesh.

Note: Internal mesh engines read ${\tt MeshDef}$ section for mesh-spacing specification.

External mesh engines -

- *Triangle* mesh: An external mesh engine which meshes 2D device with triangular finite-elements.
- *TetGen* mesh: An external mesh engine which meshes 3D device with tetrahedral finite-elements.

Note: Mesh-spacing in the given region is set by MaxEdgeLength in Region section.









(c) TetMesh

Figure: Mesh of a 2D diode generated by running the diode config file with MeshType of (a) FEM, (b) Tensor, (c) TetMesh.

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3D Mesh Types



(c) Tensor

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Onfiguring structure generator

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Python interface for structure generation

```
import device as dev
import numpy as np
# define device object
dio = dev.Device ("Diode", "FEM", "STR", 1)
xmin = -1.; xmax = 1.; xmid = 0.; ymin = -0.2; ymax = 0.2
# define RefWins
dio.setRefWin (Name="RefSi", Shape="Rectangle",
   Position=np.array ([[xmin, vmin, 0.], [xmax, vmax, 0.]]))
dio.setRefWin (Name="RefAnode", Shape="Rectangle",
   Position=np.array ([[xmax-1E-3, vmin-1E-3, 0.],
                        [xmax+1E-3, ymax+1E-3, 0, 11))
dio.setRefWin (Name="RefPDoping", Shape="Rectangle",
   Position=np.array ([[xmin, vmin, 0.], [xmid, vmax, 0.]]))
# define Regions
dio.setRegion (Name="RegSi", RefWin="RefSi", Material="Silicon")
# define Meshing
dio.setMeshDef (Name="MDefSi", RefWin="RefSi",
   Xarg=[0., 1E-4, 0.05, 1.3], Yarg=[0., 0.025, 0.025, 1.])
# define Doping
dio.setDopingDef (Name="Pdoping", RefWin="RefPDoping",
   Type="Constant", Concentration=5E16, DopantSpecies ="Boron")
# define Contacts
dio.setContact (Name="Anode", RefWin="RefAnode")
dio.createDeviceMesh () # create Mesh
dio.saveMeshData () # save Mesh
```

Argument names in *config* file and *python script* are mostly similar. Please check the manual first!

Compare DopingDef defined in config file vs. in python -

```
DopingDef+Pdoping: {
    RefWin = "RefPDoping";
    Type = "Constant";
    Concentration = 5E16;
    Dopant = "Boron";
}
```

Run the duly completed python script as follows -

>> python3 diode_str.py

- Equivalency: Python interface internally runs the software commands.
- Parametrization: Script can be reused for a similar structure.
- seamless integration: device passed as argument to the simulator objects.
- Python libraries (e.g. scikit or optimization libs) can be used in the script.

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Editing RefWins – part 1

Define ${\tt RefWin}\xspace$ objects in python as follows.

```
import mesher as m
```

```
win1 = tm.refwin("RefCyl1", "Polygon", poly, {}, {})
```

win2 = tm.refwin("RefCyl2", "Polygon", poly2, {}, {})

Boolean operations on 2D/3D RefWins -

- win1.add(win2): boolean unite
- win1.subtract(win2): boolean subtract
- win1.clip(win2): boolean intersection

Geometric transformations on 2D/3D RefWins -

- winl.translateBy(\vec{d}) and \vec{d} = tm.position(0,0,0)
- win1.scaleBy(0.5,*č*)
- winl.rotateAroundAxis(c,d,45°): point c and direction d define the axis.
- winl.mirrorByPlane(\vec{d}): \vec{d} defines plane normal

Editing 2D/3D RefWins -

- win1.chamferAt([tm.position(0,0,0)],[1])
- win1.roundAt([tm.position(0,0,0)],[0.5])



Editing 2D/3D RefWins -

- win1.offsetRefWin(2)
- win1.stretchRefWin(tm.position(2.5,0,0))
- winl.stretchRefWinAtPoint (\vec{p},\vec{d}): stretch a point \vec{p} along direction \vec{d}
- winl.limitRefWinSpan(\vec{c}_m, \vec{c}_p)



Transforming 2D RefWin to 3D -

- win.sweep2DRefWin ([ci1, ci2, ci3]): sweep along a piecewise linear path defined by [ci1, ci2, ci3].
- win1.makePrism2DRefWin(\vec{d}):sweep along \vec{d}
- winl.makePyramid2DRefWin(\vec{c}): make pyramid with "win1" as base and \vec{c} as apex point.
- winl.revolve2DRefWin($\vec{c}, \vec{d}, 360.$)



Custom etch profiles can be obtained from the mask RefWins as follows.

- win1.sweep2DMaskDepthAngle([d1,a1,d2,a2,.]): etch profile as depth, side-wall angle list.
- winl.sweep2DMaskPositionList ([\$\vec{c}_1\$, \$\vec{c}_2\$, \$\vec{c}_3\$, \$\vec{c}_4\$]): etch profile as points.

Note: The 2D mask RefWin must be in XZ plane, and the sweep direction is always along y-axis.

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Analytical doping profiles

Masked dopant implantation + diffusion creates a Gaussian distribution and lateral straggle of *error function*.

In Gaussian profile, doping at each vertex $C_i(\vec{r})$ is given by,

$$C_i(\vec{r}) = C \cdot \operatorname{erf}\left(-\left(\frac{d_{\parallel}}{\sigma}\right)^2\right) \cdot \exp\left(-\frac{1}{2}\left(\frac{d_{\perp}-\mu}{\sigma}\right)^2\right)$$

- d_{\perp} : perpendicular distance to the BaseWin.
- d_{\parallel} : lateral distance from the edges/end-points of the BaseWin.
- μ : Implantation depth from Si surface set by Depth.
- σ : Diffusion length set by DecayLength.
- C: scaling factor set by Concentration.

Alternately, Linear, Exponential, or Constant profiles can be set. Following syntax is used for creating a DopingDef.

```
DopingDef*Pdoping: {
RefWin = "RefPDoping";
Type = "Gaussian";
Concentration = 5E16; // 1/cm3
Depth = -0.1;
DecayLength = 0.2;
BaseWin = "PBaseLine";
Dopant = "Boron";
}
```







(p) Exponential



(q) Linear

Figure: Doping profiles obtained by (a) Gaussian, (b) Exponential, and (c) linear distributions. (a = b + (a = b))

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User-defined analytic doping profiles

Dopant distribution of any user-defined analytic expression is initialized in the DopingDef as follows.

```
DopingDef+Pdoping: {
    RefWin = "RefPDoping";
    Type = "Analytic";
    Concentration = 5E16;
    AnalyticExpr = "exp(-(X+0.2)*(X+0.2)/0.02)";
    Dopant = "Boron";
    ''
```

- AnalyticExpr:text containing user-defined analytic expression.
- X, Y, Z variables : x-, y-, and z- coordinates of each vertex.
- Concentration: scaling factor which internally multiplies the analytic expression.



(a) User-defined expression

Figure: Doping profiles obtained by a user-defined expression.

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```
GDSLayerDef*C1: {
    GDSFileName = "coupler.gds";
    Layer+L1: {Cell="test", Layer=0, Y=0, dY=0.2};
    Layer+L2: {Cell="test", Layer=31, Y=0.2, dY=0.0};
    Layer+L3: {Cell="test", Layer=32, Y=0.2, dY=0.0};
    Layer+L4: {Cell="test", Layer=0, Y=0.2, dY=0.2};
    DopingDef*Pdoping: {
        RefWin = "RefAll";
        Type = "Gaussian";
        Concentration = 5E16;
        Depth = 0.1;
        BaseWinGDS = ["Ci_L2", "Ci_L3"];
        Dopingt = "Boron";
    }
}
```

- GDSLayerDef: Specifies settings to create polygons from GDS mask Layers.
- Layer: Each layer creates a RefWin.
- dY: Thickness of the layer. If 0, it creates a 2D RefWin, else, a 3D RefWin.
- RefWinGDS in Region: Creates region from a 3D RefWin.
- BaseWinGDS in Doping: Sets which 2D RefWins are used as masks.



(b) Doping profile from GDS file

Figure: Doping profile in (b) using GDS mask in (a).

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Import GDS layout – region definition (in 3D device only)

```
GDSLayerDef*C1: {
  GDSFileName = "coupler.gds";
  Layer+L1: [Cell="test", Layer=0, Y=0, dY=0.2};
  Layer+L2: [Cell="test", Layer=31, Y=0.2, dY=0.0];
  Layer+L3: [Cell="test", Layer=32, Y=0.2, dY=0.2];
  Layer+L4: {Cell="test", Layer=0, Y=0.2, dY=0.2};
  }
  Region*RegSi: {
    RefWinGDS = ["C1_L2", "C1_L3"];
    Material = "Silicon";
  }
  Region*RegOxTop: {
    RefWinGDS = ["C1_L1"];
    Material = "Oxide";
  }
}
```

- GDSLayerDef: Specifies settings to create polygons from GDS mask Layers.
- Layer: Each layer creates a RefWin.
- dY: Thickness of the layer. If 0, it creates a 2D RefWin, else, a 3D RefWin.
- RefWinGDS in Region: Creates region from a 3D RefWin.
- BaseWinGDS in Doping: Sets which 2D RefWins are used as masks.



(a) GDS file of Silicon wave-guide



(b) Silicon wave-guide structure

Figure: Silicon wave-guide structure in (b) using GDS mask in (a).

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GUI - Main window



File	View	Edit	Add Shape	Set Shape A
ŝ	New			Ctrl+N
	Open			
	Save			
	Save A	s STE	P	
	Import	GDS	File	
	Export	Pytho	on Script	
ſø	Close			

(b) File menu

- New Open new circuitdraw window.
- Open File Selected '*.qstr' file opened in a new window.
- Save (As) Current (New) '*.qstr' file is stored.
- Save As STEP Save current structure as a STEP file.
- Import GDS File Import a layout file in GDS format.
- Export Python Script Export python script which can generate the structure.

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	Vie	W	Edit	Add	Shape	Se
>	C	D	rag So	reen		
,		Ζ	oom T	o Fit		
	~	3	D			
ıi		E	x			
		R	uler			
		M	lesh			
		M	lask			
		P	rocess			

(c) File menu

To change screen viewpoint -

- Middle Mouse Button: Drag screen.
- Right Mouse Button: Rotate camera view-point.
- Drag screen : (if middle mouse button is not available) Drag screen.
- Zoom To Fit : Click to zoom the structure to fit the entire window.
- 3D : Set given structure as a 3D structure. It cannot be changed mid-way.
- Ex : Activate 'exact coordinates'. When active, any shape drawing action would prompt a dialog box to specify x,y,z coordinates of the point.
- Ruler : Activate it. Click start point of the ruler and end point to measure distance.
- Mesh : Click to display/hide mesh generated by the mesher.

Edit Add Shape Set Shape . ▷ Move □ Copy ② Delete ▲ Flip	As Create Mesh Add Process At Ctrl+M Ctrl+C Del Del Ctrl+C
Boolean Operation Select Shapes Round Selected Chamfer Selected Clear Selection	Unite Intersect Subtract
Image: Head Stretch Image: Offset Image: Prism from 2D Shape Image: Pyramid from 2D Shape Revolve 2D Shape	

(d) Edit menu

- Move, Copy: Activate it. Click on shape to be moved/copied and click where to place it.
- Delete : Activate it. Click on the shape to delete.
- Flip: Activate it. Click on the shape to be flipped w.r.t. guide-plane at given intercept.
- Select : Activate it. Click on shapes to be selected.
- Clear Selection: Click on it to clear all selected shapes.
- Boolean operation: After selecting the shapes, click on the operation.
 - Unite : Join all selected shapes and store in the first shape.
 - Intersect : Find common areas of selected shapes and store in the first shape.
 - Subtract : Subtract selected shapes from the first shape.
- Round Selected, Chamfer Selected: Round/chamfer all corners of selected shapes with the given rounding/chamfer radius (in μ m).
- Stretch: Activate it. Click on the shape to be stretched at the point where to stretch. Specify stretch distance.
- Offset : Activate it. Specify offset distance. Click on the shape to be offset.
- Prism/Pyramid from 2D Shape : Activate it. click on the 2D shape and click at the apex point. A pyramid/prism would be created.
- Revolve 2D shape: Activate it. Click on the 2D shape. Fix location of axis of revolution.

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Ado	d Shape Set Shape As Cre	eate
P	Segment	p
0	Regular Polygon	
23	, Polygon	
	Rectangle	
0	Circle/Ellipse	
\heartsuit	Cuboid	
0	Cylinder	
4	Cone	
⊕	Sphere/Ellipsoid	
۵	Prism	
Φ	Pyramid	
	Wedge	
\bigcirc	Convex hull	
	Convex hull from file	
	From Last Selected	
	Load STL/BREP/IGES	

(e) Add Shape menu

To add a RefWin of a given shape, activate its icon by click. Then perform -

- Segment : Click on two opposite points of the segment.
- Regular Polygon, Rectangle, Ellipse: Click on two diagonally opposite points of the axis-aligned rectangle to add the respective shape inscribing the rectangle.
- Polygon: Click on the consecutive corners of the polygon. Double click on the last corner to add polygon.
- Cuboid, Cylinder, Cone, Ellipsoid, Prism, Pyramid, Wedge: Click on two diagonally opposite points of the axis-aligned rectangle to add the base of the respective shape. Then click on the third point (not in the same plane) to specify height of the shape.
- Convex Hull: Click on the points of the convex hull. Double click on the last point to add convex hull.
- Convex Hull From File: Load points of the convex hull from a csv file. It has N x 3 table. Each row has one point and x,y,z co-ordinates are stored in 3 columns.
- From Last Selected: Select a shape, an edge, or a face. Then click to convert that item to a RefWin.
- Load STL/BREP/IGES: Load the files in the specified format to create a new RefWin.

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GUI - Set Region

Sel	:Region 🛛 🔇
Reg. Name:	Reg1
Material:	Silicon 🔹
RefWins:	Sh_0 •
Max. area o	f elements:
Bulk:	0.1
Interface:	0.05
Doping Refir	nement Params:
Doping Grac	lient:
Max. value	
Min. value	
Element are	a constraint for:
Max. grad.	
Min. grad.	
[● <u>C</u> ancel

(f) Set Region menu

Set Shape As... Create Me Region Mesh Refinement Contact Doping Definition

(g) Set Shape As menu

To set a Region from one or more RefWins (shapes) -

- Edit \rightarrow Select the desired shapes.
- Click Set Shape As \rightarrow Region to open the dialog box.

Region dialog box is described below -

- Reg. Name : Set name of the region.
- Material: Set material from available materials.
- RefWins : Names of the selected RefWins are listed here.
- Max area of elements: Maximum area of elements in bulk and at interface for meshing using Triangle or TetGen mesher.
- Doping gradient: max and min gradient and their corresponding element area constraints. Element area is linearly interpolated between maximum and min gradients (only valid for meshing using Triangle or TetGenmesher).

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Name:	M1	RefWins:	Sh_0 ▼
Refinements:	Along X	Along Y	Along Z
Center:	0.1	0.1	0.1
Min spacing:	0.1	0.1	0.1
Max spacing:	0.1	0.1	0.1
Increment by:	1	1	1
Quad/Oct-Tree	Doping Gra	dient Cutoff:	

(h) Set Mesh Definition

To set a MeshDef from a RefWin -

- Edit \rightarrow Select the desired shape.
- Click Set Shape As \rightarrow Mesh Definition to open the dialog box.

Mesh Definition dialog box is described below -

- MeshDef Name: Set name of the mesh-definition.
- RefWins: Names of the selected RefWins are listed here.
- Refinements along X, Y, and Z direction are specified in respective columns.
- Center : Center of the refinement point
- Min spacing: spacing at the center.
- Max spacing: max spacing in the refinement box.
- Increment by: As one moves away from Center, spacing increases from min to max. Mutiplying factor is set in Increment by.
- Doping gradient Cutoff: Quadtree or octtree leaves are split if doping gradient along a side is more than this value.

Note: This mesh definition box is used only in quadtree (2D) or octtree (3D) meshers.

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Set Doping	Definition 隆	3
Name:	Dop1	
RefWins:	Sh_0 -	
Туре:	Constant 🔹	
Dopant:	Boron 💌	
Set BaseWin:	•	
Conc.	1E16	
Depth		
Decay Length		
Analytic Expr.		
۲	Cancel	

(i) Set Doping Definition

To set a MeshDef from a RefWin -

- Edit \rightarrow Select the desired shape.
- Click Set Shape As \rightarrow Mesh Definition to open the dialog box.

Doping Definition dialog box is described below –

- DopingDef Name : Set name of the doping definition.
- RefWins : Names of the selected RefWins are listed here.
- Type : Set the type of definition Gaussian, constant, analytic, etc.
- Dopant : Specify dopant among available ones.
- Set BaseWin: Set basewin for the doping profile
- Conc : Set peak concentration (cm⁻³)
- Depthand Decay Length: For Gaussian and Exponential profiles, set distance of peak from basewin and its decay length.
- Analytic Expr.: For analytic profiles, define analytic expression.



(j) Set Contact

To set a Contact from a RefWin -

- Edit \rightarrow Select the desired shape.
- Click Set Shape As \rightarrow Contact to open the dialog box.

Contact dialog box is described below -

- Contact Name : Set name of the contact.
- RefWins : Names of the selected RefWins are listed here.

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Create Mesh Add Proces Tensor Mesh Quad-/Oct-tree Triangle/CGAL TQMesh/TetGen

(k) Set Contact

- Once all the regions, mesh definitions, doping definitions, and contacts are set, a mesh can be created.
- Click Create Mesh and then choose the desired mesh engine to perform meshing.
- On succesfull meshing, the Mesh mode is activated and mesh is shown in the drawing board. To toggle to structure view, deactivate Mesh mode.

Following meshing options are available.

- Tensor mesh : Rectangular (2D) or Cubic (3D) meshing can be performed.
- Quad-/Octtree : FEM mesh is created using quadtree (2D) or octtree (3D) algorithm.
- Triangle/Tetgen : FEM mesh is created using Triangle or Tetgen package.

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3D Shapes	Regions	Mesh	Doning	Contac	ts
Id	Name		Material	Sho	w/Hide

Shapes Side-pane

- Shapes tab displays all the shapes as well as entities (regions, mesh defs, etc.) which have been added to the structure generator. They are displayed in different tabs in the table.
- To display/hide a shape linked to the given entity, click on the check-box in the last column of the table.
- Order in Regions as well as Contacts tab is important. If there is an overlap, regions/contacts added later replace the region/contact added before.
- Entity order can be changed by clicking on it and click move up/down.
- Delete entity by clicking on it and click Remove

Active GDS F	ile:		
		avout to structu	ire - l
(r			ile - I
(r Y-intercept:	n) GDS 1	Thickness dY:	
(r Y-intercept: Mask X-min:	-1E3	Thickness dY: Mask X-span dX:	2E3

- Layers defined in imported layout files are listed in this tab. The files can be selected from the drop-down list.
- Check/uncheck the check-box to show/hide the layout of that layer.
- Set the parameters Y intercept, Thickness, mask Xmin, dX, Zmin, dZ.
- Click Create RefWin to add a RefWin as per the parameter specifications.

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The structure generator supports creating -

- A 2D/3D device from a rectangle/cuboid, polygon/polyhedron, ellipse (2D), ellipsoid, cylinder, or cone (3D).
- Boolean operations, transformations, and sweeps of 2D/3D devices.
- Doping definitions of analytic profiles such as Gaussian, exponential, linear, or user-defined.
- Mesh refinements globally or in specific regions.
- Python interface for convenient scripting and integration.
- Import GDS layout file to create masks for doping, etching, or deposition.
- FEM-mesh, Tensor-mesh, *Triangle* mesh, and, *TetGen* mesh.
- A graphic-user-interface for convenient creation of the structure.

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- Onfiguring structure generator
- Optimize Python interface
- Editing RefWins
- G Analytical doping profiles
- Importing GDS layouts
- Graphical user interface
- 8 Conclusion

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The End

Questions? Comments?

