HDF Vset File Format for Persistent Storage of Semiconductor Simulation Data

Dan Yergeau, Zakir Sahul, Robert Dutton
Integrated Circuits Lab
Stanford University
Stanford, California 94305

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1.0 Overview

This document discusses VGeMesh (vee-gee-mesh), a file structure using HDF Vset[1] as an efficient format for storing semiconductor simulation data sets. The purpose of the standardized format is to facilitate data exchange between various simulators and to provide an unstructured mesh representation that is usable by high-end visualization tools. The proposed format provides a minimal representation standard for unstructured meshes and geometry. The organization of data is designed to be flexible and to allow additional representations (e.g. tree-structured meshes, mask or process flow) to be added while still remaining backward compatible with existing applications. It should be emphasized that an application can use any of a number of different data structures to represent the structure and the fields on the structure. Typically, an application will store a geometry, an unstructured mesh, and several fields interpolated on the unstructured mesh. However, it may only store an unstructured mesh or only the geometry. The access mechanisms provided by HDF Vset provide easy and efficient retrieval of only the data that the simulation tool understands.

HDF Vset provides low-level hierarchical management of homogeneous data sets in a similar fashion to a Unix file system. The concepts of directories and files map into Vgroups and Vdata in HDF Vset. Actual data is contained in Vdata. Related Vdata are hierarchically grouped together to form Vgroups. VGeMeshVGeMesh defines the organization of the hierarchy and the naming conventions and data structures to be used to represent semiconductor simulation data.

It must be emphasized that this document describes a format that is fully extensible. Backward compatibility assures that any applications that use the standard will not be affected when a new representation is defined.

2.0 VGeMesh File Layout

The general layout of a VGeMesh file is shown in Figure 1. A VGeMesh file consists of a required **Documentation** Vgroup and a sequence of one or more *Frame* Vgroups. Each frame consists of a

1. HDF Vset source and documentation are available via anonymous ftp from ftp.ncsa.uiuc.edu

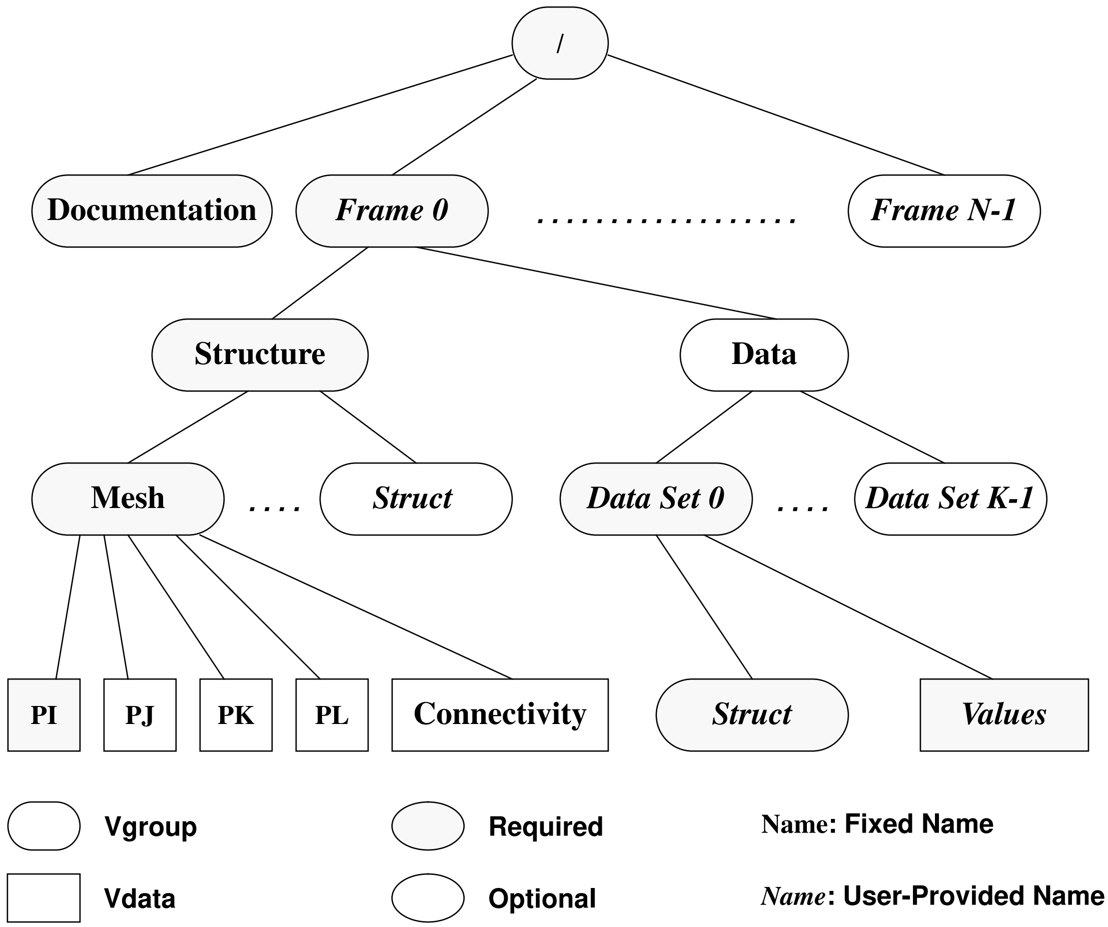


FIGURE 1 HDF-Vset file hierarchy for semiconductor simulation data.

required **Structure** Vgroup and an optional **Data** Vgroup. The **Structure** Vgroup may provide an unstructured mesh, geometry, or a tree-structured mesh. The **Data** Vgroup is used for storing scalar and vector data defined at the nodes of a given unstructured mesh. The naming conventions for the Vgroups and Vdata in the hierarchy and data structures are discussed in detail in the following sections. These descriptions assume that the reader is familiar with the HDF Vset hierarchy and data access methods.

The following notation is used throughout this document: Bold typeface is used for predefined names. The context will indicate whether a name is for a Vgroup or a Vdata. For example, **Documentation** is a predefined Vgroup. Italics are used to indicate Vgroups or Vdata whose names are supplied by the application (i.e., they are not predefined). An example of such Vgroups is the *Frame* Vgroup.

2.1 Documentation

The **Documentation** Vgroup provides a means of documenting both the entire file as well as any component of the data set. The top level, *Frame*, **Structure** or **Data** Vgroups may have a **Docu-**

mentation Vgroup contained within. A documentation Vgroup is identified as any Vgroup with class name **Documentation**. There are three predefined Vdata in the **Documentation** Vgroup - **Name**, **Creator**, and **Notes**. The first Vdata, **Name**, holds the name given to the data set and is limited to 255 characters. The second Vdata, **Creator**, holds the name and version of the tool that created the data set, and is intended to be used as a hint to the data sets contained within. It is also limited to 255 characters. The last Vdata, **Notes**, is open to a general description of the data, its simulation techniques, and any other information of general interest about the simulation data. It has no length restriction.

2.2 Frames

Any other Vgroup at the top level with class name **Frame** is a frame. Frames provide a means for sequencing of groups of simulation data. For example, in semiconductor process simulation, the frames may represent the state of the wafer after certain processing steps. At least one frame must be present and each of the frame Vgroups must have a unique name.

2.3 Structure

A Vgroup named **Structure** under a *Frame* Vgroup stores the meshes or geometry in each frame. A **Structure** Vgroup must have at least one Vgroup that is one of **Mesh**, or **Geometry**. The **Mesh** Vgroup will store an unstructured mesh and the **Geometry** Vgroup will store the structure's geometry.

2.4 The Mesh Vgroup

The **Mesh** Vgroup stores all information needed to store and construct an unstructured mesh. It contains Vdata that store the coordinates of the nodes in the mesh and their connectivity to form elements in the mesh. Optionally, it may contain a Vdata to contain local structuring (defined below). It may also contain any other Vdata or Vgroups to contain attributes that are necessary for persistent storage and retrieval of data. This includes material attributes for elements.

2.4.1 Coordinates

Vdata with the names **PI, PJ**, **PK**, and **PL** represent coordinates of the nodes of the mesh. **PI**, **PJ**, and **PK**, represent x, y, z coordinates respectively in a right handed coordinate system. **PL** is to be used for time. Numbering within a coordinate Vdata is required to start with zero (0).

2.4.2 Predefined Connectivity

An unstructured mesh is represented by an element list. Each element consists of a set of points that connect to form it. The name of the Vdata containing the connectivity of each element is used to determine the types of elements in the mesh. A useful subset of Vdata names and meshes are defined. They are as shown in Table 1. The format allows for mixed meshes (i.e. meshes composed of several different types of elements), provided that all elements are a degenerate case of some higher order element, and are of the same dimension. No distinction is made between surface or volume meshes. Both can be represented using this format..

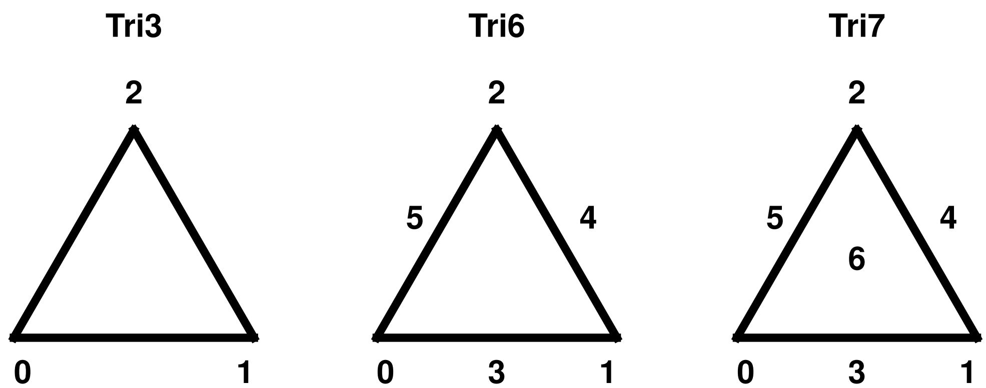
TABLE 1. Predefined Vdata for mesh connectivity

Vdata Name	Type of element in mesh
Edge2	2 noded edges
Edge3	3 noded edges
Tri3	3 noded triangles
Tri6	6 noded triangles
Tri7	7 noded triangles
Quad4	4 noded quadrilaterals
Quad9	9 noded quadrilaterals
Tetra4	4 noded tetrahedra
Tetra10	10 noded tetrahedra
Hexahedron8	8 noded hexahedra
Hexahedron20	20 noded hexahedra

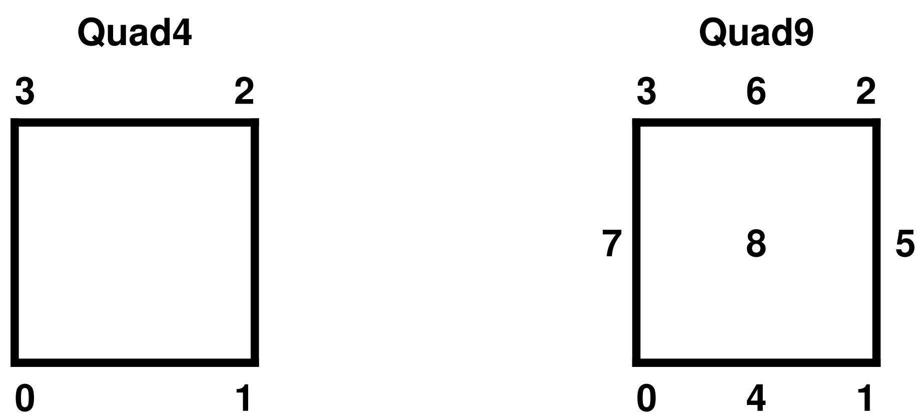
In the following figures, numbers refer to local nodes of an element. Each connectivity list consists of a two dimensional array of the number of elements by the maximum number of nodes per element. Entries in this array are integers indexing into the coordinate arrays, assuming that the first element in the coordinate arrays is element 0. The connectivity is stored fully interlaced, varying local nodes most rapidly. For a degenerate element, the corresponding node is -1 (minus one). Although mapping of coordinates is unspecified, the convention chosen should be consistent - always clockwise or counterclockwise.

2.4.2.1 Edges

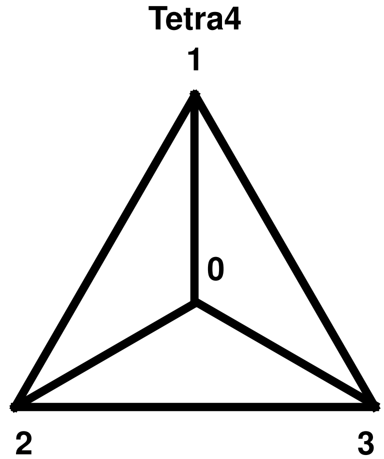
2.4.2.2 Triangles

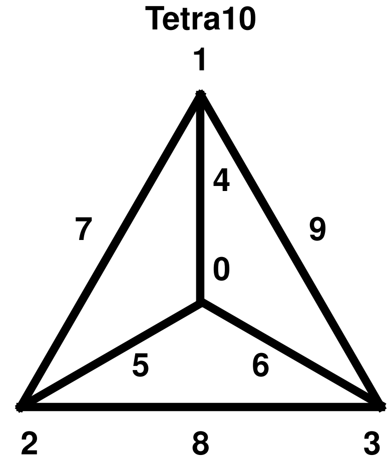


2.4.2.3 Quadrilaterals

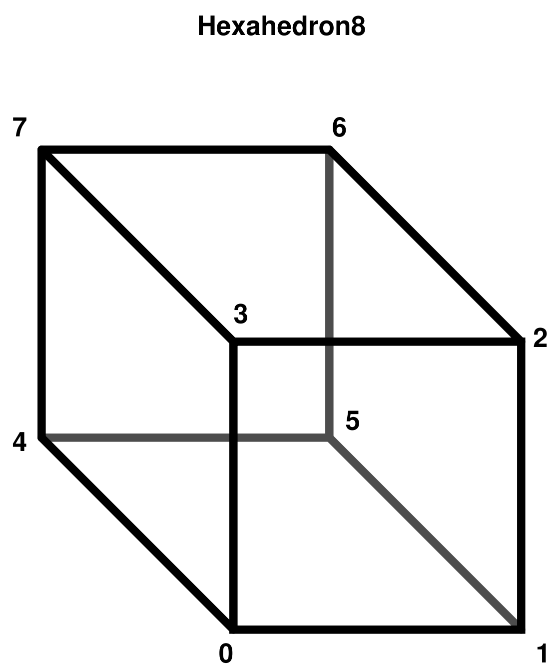


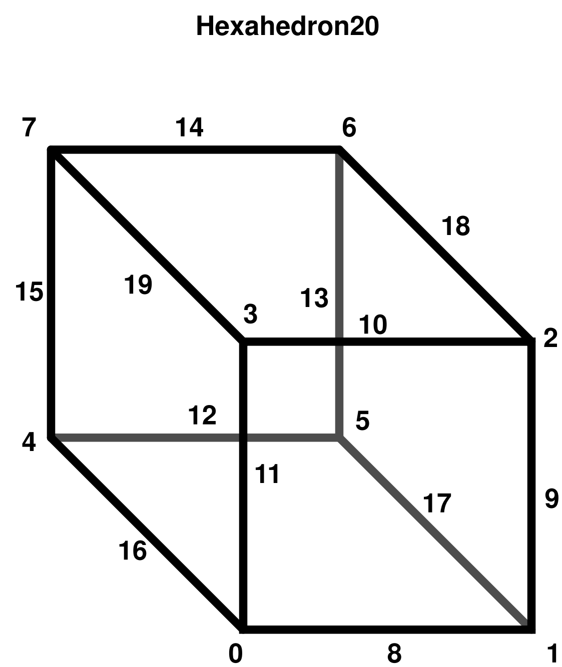
2.4.2.4 Tetrahedra





2.4.2.5 Hexahedra





2.4.3 Auxiliary Connectivity

Auxiliary connectivity information may be used to store local element structure such as neighbor information and boundary conditions. As such, the Vdata **AuxiliaryConnectivity** is predefined. For 2D elements, this Vdata contains neighbors that share the same edge. For example, if a quad is defined to be connected between nodes 4, 9, 13, and 17. The **AuxiliaryConnectivity** Vdata for the element will contain four entries corresponding to element numbers that share the edge connecting each of: nodes 4 and 9, nodes 9 and 13, nodes 13 and 17, and nodes 4 and 17. This scheme is illustrated in the example. For 3D elements, the neighbor number semantics are defined in Tables 2 and 3. The faces refered to in the tables are defined by the element node numbering in the element figures above. Furthermore, the number of neighbors for each element is equal to the number of edges or faces of the element. Thus, all triangles (3 noded, 4 noded, 6 noded or 7 noded) have three neighbors.

TABLE 2. Element neighbor numbering semantics for tetrahedra meshes

Neighbor #	Shared face
0	[012]
1	[023]
2	[031]
3	[123]

TABLE 3. Element neighbor numbering semantics for hexahedra meshes

Neighbor #	Shared Face
0	[0123]
1	[0154]
2	[0374]
3	[1265]
4	[2673]
5	[4567]

If the element is along a boundary and does not have a neighbor, then this Vdata entry can be used to define boundary conditions. For process simulation meshes, the neighbor numbers are used for specifying the commonly encountered boundary conditions and are listed in Table 4 For device simulation, negative numbers for neighbors indicate electrode numbers at the edge (without the minus sign). An electrode number of -1024 specifies an open electrode with an infinite resistance.

TABLE 4. Specification of boundary conditions in process simulation

Neighbor #	Boundary Condition
-1022	Reflecting Surface
-1023	Exposed Surface
-1024	Backside Surface

Neighbor information can be built from scratch from a fully unstructured mesh without a **AuxiliaryConnectivity** Vdata. However, for applications that do not store the geometry of the device, the **AuxiliaryConnectivity** Vdata is the only way to specify boundary conditions.

2.4.4 Vdata for storing material data

For both device and process simulation, elements are defined over different materials. Material data are stored in a separate Vdata called **Material** under the **Mesh** Vgroup. Common materials and their corresponding material numbers are defined as in Table 5 .

TABLE 5. Predefined material numbers to be used in the Material Vdata

Number	Material
0	Gas (ether)
1	Silicon Dioxide (SiO2)
2	Silicon Nitride (Si3N4)
3	Silicon (Si)
4	Polysilicon
5	Silicon oxynitride
6	Aluminum
7	Photoresist
8	GaAs
9	General Semiconductor
10	Silicon Germanium (SiGe)
11	Aluminum Gallium Arsenide (AlGaAs)
12	Aluminum Indium Arsenide (AlInAs)
13	Indium Arsenide InAs
14	Gallium Indium Arsenide Phosphide (GaInAsP)
15	Sapphire
16	General insulator

Compound materials that have fractional compositions (e.g. $Al_xGa_{1-x}As$) need to store the composition in a separate Vdata. Thus, two Vdatas - **MaterialXComposition** and **MaterialYComposition** are predefined.

2.4.5 Example

The example illustrated in Figure 2 shows the use of VGeMesh for storing an unstructured mesh. Numbers within parentheses represent coordinate values. Numbers within brackets represent element numbers. Numbers next to black dots represent node numbers. Note the use of degenerate elements to store solution values for Gas nodes. This is useful for storing ambient concentrations of impurities for process simulation. However, this scheme requires the use of elements to access solutions because nodes in the coordinates list will be duplicated.

2.5 The Geometry Vgroup

The geometry is defined as a hierarchy of points, edges, boundaries, and regions in 2D and points, edges, boundaries, surfaces and volumes in 3D. The following Vdata names are predefined for

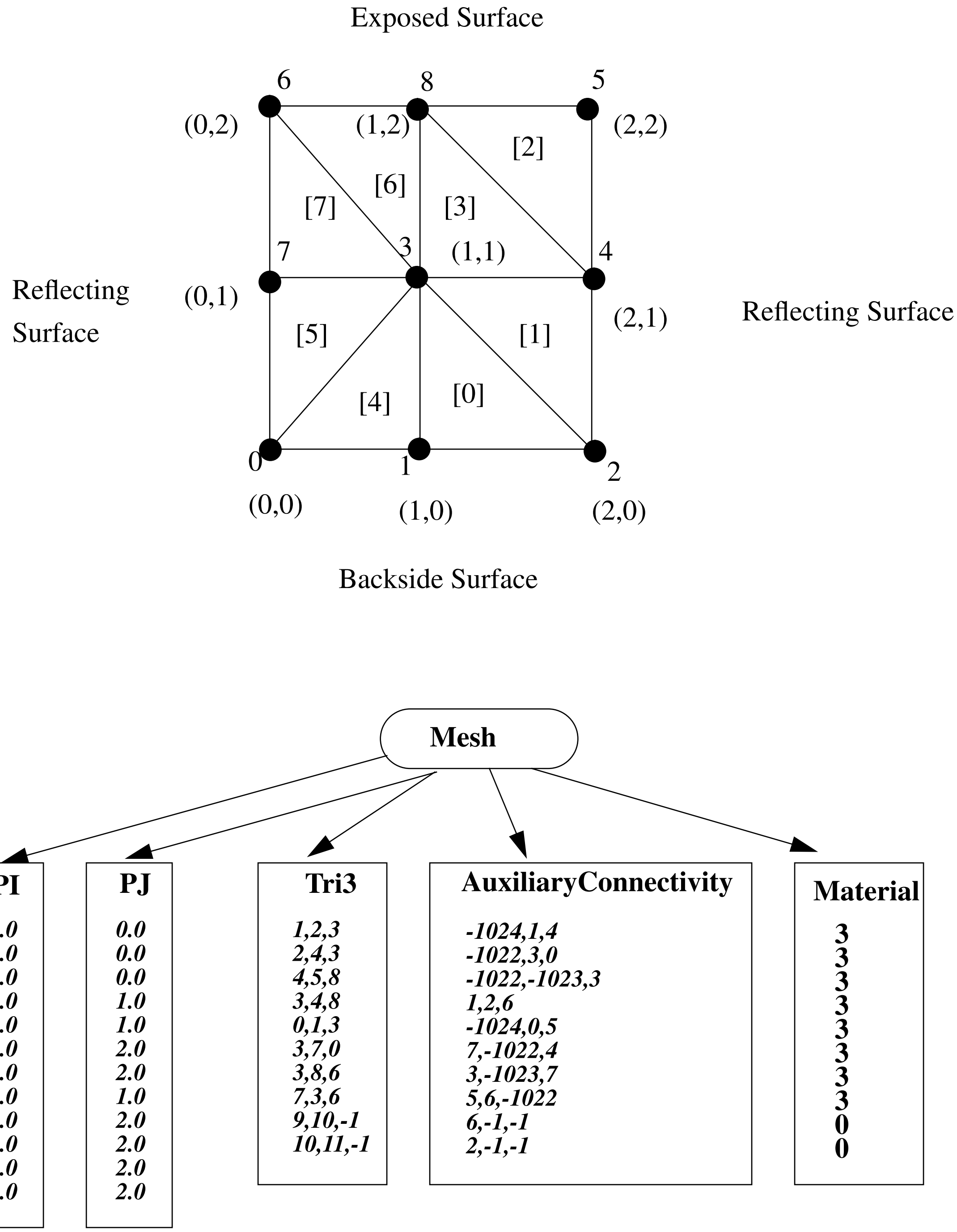


FIGURE 2 Example VGeMesh file for storing unstructured meshes.

storing geometries: **PI**, **PJ**, **PK**, **Edge**, **Boundary**, **Region** and **Volume**. **PI**, **PJ** and **PK** are used to store the coordinates of the spatial points identical to their use in the **Mesh** Vgroup.

Edge Vdata is an integer dataset containing indexes into the coordinates Vdata for the starting and ending points of an edge. There are thus two indices for each edge. **Boundary** Vdata ia an integer dataset that contains an ordered listing of edge indices that comprise the boundaries. Clockwise or counterclockwise sense of the ordering is left unspecified. Since a geometry normally contains many boundaries each with a different number of edges, a **BoundaryNoofEdges** Vdata is defined to act as an index into the **Boundary** Vdata. For example, if a geometry contains 3 boundaries with 34, 9, and 15 edges, **BoundaryNoofEdges** will be a Vdata with three elements: 34, 9 and 15. **Region** and **Volume** Vdata are defined similarly with the auxiliary Vdata **RegionNoofBoundaries** and **VolumeNoofRegions**. This scheme allows for a compressed sparse storage mechanism. Please see the example below for further elucidation.

Other Vdata may be defined as needed to contain other attributes of the objects that comprise the geometry. Materials are defined over regions and material data are stored in Vdata called **Material.** The format and numbering of the **Material** and optional **MaterialXComposition** and **MaterialYComposition** are identical to their use in the **Mesh** Vgroup. Boundary conditions are specified on edges using the predefined Vdata **BoundaryCondition**. The same numbering mechanism for exposed, reflecting and backside boundary conditions and electrode information is used as described for the **Mesh** Vgroup.

2.5.1 Example

The example illustrated in Figure 3 shows the use of VGeMesh for storing a geometry. Numbers within parentheses represent coordinate values. Numbers next to black dots represent node numbers. Numbers within brackets represent edge numbers. Numbers within curly braces represent boundary numbers. Numbers delimited by asterisks are region numbers. There are two regions. and region one has two boundaries.

2.6 Data

Data is stored under a Vgroup named **Data** under a *Frame* Vgroup. It groups the data sets in each *Frame*. If present, a **Data** Vgroup must have at least one data set Vgroup.

2.7 Data Sets

A *Data Set* Vgroup is any non-Documentation Vgroup under the Data Vgroup. It must contain a Vgroup which is a link to one of the meshes in the same frame's **Structure** Vgroup. It must also have a *Values* Vdata containing values at the nodes of the given mesh. This Vdata must contain the same number of elements as the coordinate Vdata in the mesh. The names **Scalar**, **Vector2**, and **Vector3** are reserved for *Values* Vdata. Each of these contain floating point values. The vector types are stored fully interlaced and provide data consistent with the ordering of the coordinate axes (i.e. **PI**,**PJ** or **PI**,**PJ**,**PK**, respectively). Other value representations may be added (e.g. magnitude and phase for a complex number, tensors, etc.).

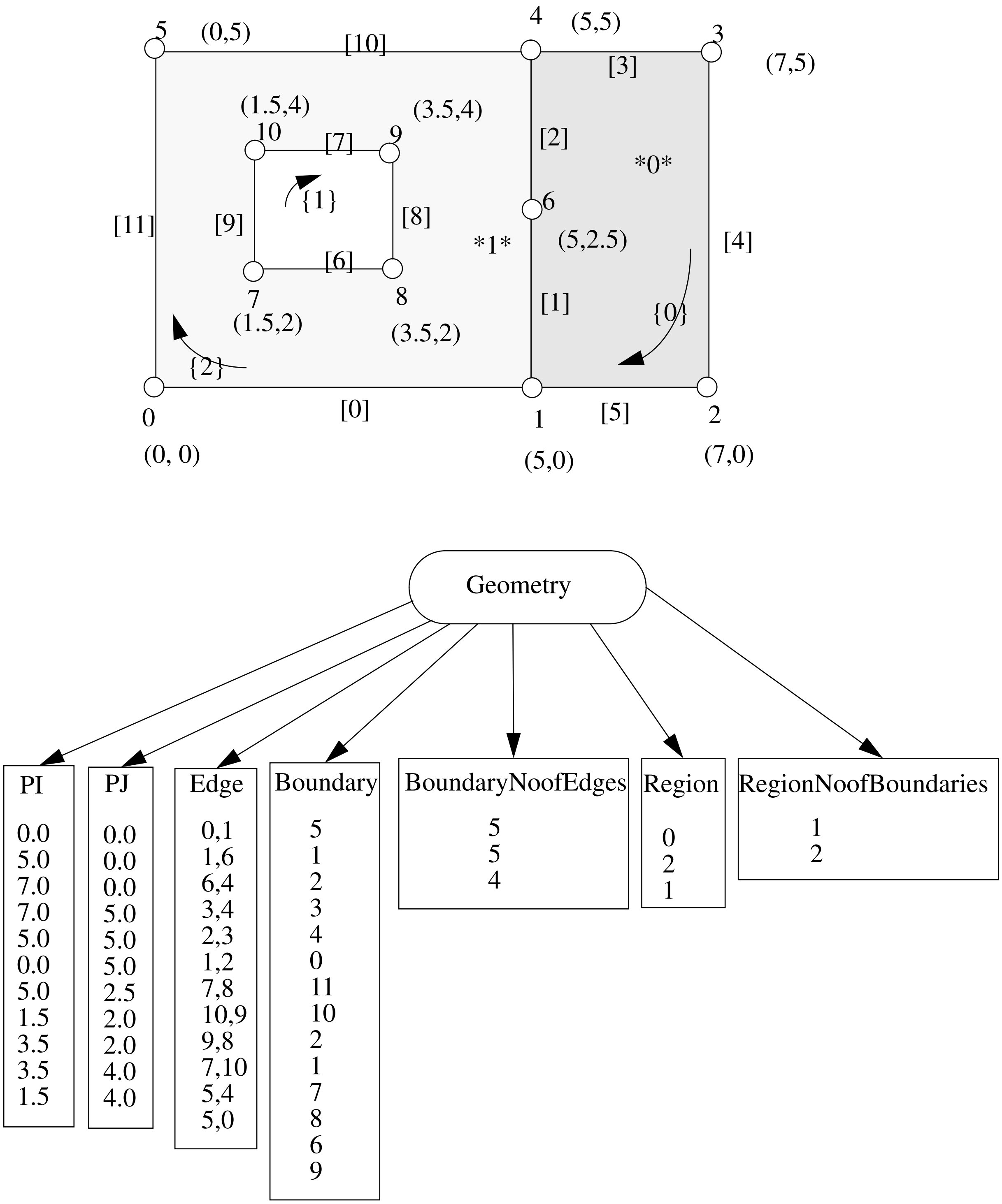


FIGURE 3 Example VGeMesh structure for storing the geometry.

The following list enumerates predefined *Data Set* Vgroup names for quantities of interest in semiconductor device simulation. None of these is required.

NetDoping	**TotalDoping**
TotalDonorDoping	**TotalAcceptorDoping**
DonorTrapConcentration	**AcceptorTrapConcentration**
DonorTrapLevel	**AcceptorTrapLevel**
ElectronMobility	**HoleMobility**
NetRecombination	**RadiativeRecombination**
SHRRecombination	**AugerRecombination**
ElectricPotential	**ElectricField**
ElectronQuasiFermiLevel	**HoleQuasiFermiLevel**
ElectronLifetime	**HoleLifetime**
ElectronConcentration	**HoleConcentration**
ConductionCurrent	**DisplacementCurrent**
ElectronCurrent	**HoleCurrent**
TotalCurrent	**LatticeTemperature**
ElectronTemperature	**HoleTemperature**
DielectricConstant	**ElectronAffinity**
ConductionDensityOfStates	**ValenceDensityOfStates**
ConductionBandOffset	**ValenceBandOffset**
Composition	**Bandgap**
ImpactIonization	

The following list enumerates predefined *Data Set* Vgroups quantities of interest in semiconductor process simulation. None of these is required.

InterstitialConcentration	**VacancyConcentration**
InterstitialTrapConcentration	**ElectricPotential**
ElectronConcentration	**HoleConcentration**
Velocity	**Stress**

In addition to the quantities listed above, impurity concentrations are named by either *Impurity*-**ActiveConcentration** or *Impurity***ChemicalConcentration**, where *Impurity* is the name of the element. For example, **BoronChemicalConcentration** and **BoronActiveConcentration** are Vdata for storing chemical and active concentration values of Boron.