# The Overture Grid Classes Users' Guide, Version 1.0 

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#### Abstract

Overture is a library containing classes for grids, overlapping grid generation and the discretization and solution of PDEs on overlapping grids. This document shows how the Overture grid classes may be used. The primary classes described are the MappedGrid, GridCollection and CompositeGrid classes. These classes hold the geometry arrays required by PDE solvers such as the vertex (grid vertices), vertexDerivative (jacobian derivatives), and vertexBoundaryNormal (normals on the boundary), etc. The geometry arrays can be optionally generated as required by the application. The grid classes have support for multigrid levels and for adaptive mesh refinement. While reading this users' guide, it may be useful to have a copy of the reference manual " The Overture Grid Classes, Reference Guide" at hand. Both this users' guide and the reference manual may be found on the Overture home page.


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## 1 Introduction

The Overture framework contains C++ classes that describe grids for the discretization of partial differential equations on complex domains in one, two and three dimensions. While most of our work until now has been in the area of finite-difference and finite-volume methods using boundary-fitted curvilinear grids and overlapping collections of such grids, we anticipate supporting additional types of grids and the methods that use them. The Overture grid classes include classes for single grids and classes for collections of grids. The single-grid classes are related to each other through the C++ inheritance mechanism. The base class is GenericGrid (§2), which actually contains no geometric data. The class MappedGrid ( $\S 3$ ) is derived from GenericGrid and is used to describe curvilinear grids. It contains the geometric data normally required for the implementation of finite-difference and finite-volume methods. The collections of grids are also related to each other through inheritance. The base class for collections of grids is GenericGridCollection ( $\S 4$ ), which contains a collection of GenericGrids. The class GridCollection $(\S 5)$ is derived from GenericGridCollection, and contains a collection of MappedGrids. All other Overture grid classes that contain collections of MappedGrids are derived from GridCollection. In particular, the class CompositeGrid ( $\S 6$ ) is derived from GridCollection. All of the Overture grid classes are reference-counted, using the envelope-letter paradigm. To support this, the base grid classes GenericGrid and GenericGridCollection are derived from the base class ReferenceCounting (Appendix A). All of these classes are described in this document.

## 2 Class GenericGrid

Class GenericGrid is the base class for all of the Overture single-grid classes. By itself it does not contain any geometric data. It is useful only as a base class for other grid classes that contain data to describe particular kinds of grids. We envision deriving from GenericGrid separate classes for structured and unstructured grids, and perhaps for other kinds of grids that we have not yet anticipated. For example, the class MappedGrid ( $\S 3$ ) is derived from GenericGrid in order to describe curvilinear structured grids. GenericGrid is derived from class ReferenceCounting (Appendix A), which provides a mechanism for implementing the envelope-letter paradigm for reference-counted objects. This allows several GenericGrids to share the same data, in such a way that the data are deallocated only when the last GenericGrid that uses the data is destroyed, due either to its being deleted or to its going out of scope.

### 2.1 Data-sharing between GenericGrids

Example 2.1 shows several ways that a GenericGrid can be made either to share data or to contain a separate copy of the data of another grid. The copy constructor can be used to construct a "shallow copy" of another grid, so that the two grids share the same data. The three forms shown in Example 2.1 for the use of the copy constructor to construct a shallow copy are equivalent and may be used interchangeably. An existing grid can also be made to become a shallow copy of another grid by using the reference() member function, as shown in the example. The example also shows several ways to make a "deep copy," in which data are copied from one grid to another when the two grids do not share data. First, the copy constructor may be used, with the second argument set to DEEP, to construct a copy of a grid with separate data all set equal to that of the original grid. Second, operator=() may be used to copy one grid to another existing grid. This will of course also modify any other grids with which the latter shares data. Third, a deep copy can be accomplished by using the reference() member function, followed by using the breakReference() member function, as shown in Example 2.1. By contrast to the use of operator=(), this method does not modify any other grids with which the grid originally shared data before the call to reference(). The member functions operator $==()$ and operator! $=()$ answer the question of whether two GenericGrids are references to the same grid, in the sense that they share the same data. This test is fast and easy, but is not equivalent to checking whether all of the data of two distinct grids are equal. All of the functions shown in this example are available in derived classes such as MappedGrid. In some cases they may be called directly, as for operator $==()$ and operator!=(); in some cases as virtual functions, as for breakReference(); and in other cases as overloaded functions with arguments of the appropriate derived types, as for the copy constructor, operator=() and reference().

```
#include "GenericGrid.h"
void example(const GenericGrid & g0)
{
    GenericGrid // Construct some grids.
        g1,
    // g1 uses the default constructor.
```

```
            g2 = g0, g3(g0), g4(g0, SHALLOW), // g2, g3 and g4 are "shallow copies" sharing data with g0,
            g5(g0, DEEP);
    g1.breakReference();
    g1 = g0; assert(g1 != g0); // Now g1 is a "deep copy" of g0.
    g1.breakReference}();
    g1.reference}(g0); assert(g1 == g0); // Now g1 is a "shallow copy," sharing data with g0.
    g1.breakReference(); assert(g1 != g0); // Now g1 has a separate "deep copy" of its old data.
}
```

Deep and shallow copies of GenericGrids

### 2.2 Geometry management

Some member functions of class GenericGrid are used to manage the geometric data of a grid. Several of these member functions are overloaded in derived classes such as MappedGrid (See also the discussion in §3.1.) They are defined in the base grid class in order to provide a consistent interface independent of the particular derived class. They use the C++ virtual function mechanism in order to manage the geometry of derived classes in situations where only the base grid class name is known. The member function computedGeometry () returns a mask that indicates which geometric data have been computed and are up-to-date. Since class GenericGrid contains no geometric data, this mask is meaningful only for an object belonging to a derived class. The member function geometryHasChanged() is used to mark geometric data out-of-date. It takes as an optional argument an integer mask that indicates which geometric data have become out-of-date. This function has a default argument value that indicates all geometric data, including the data of any derived class. Before attempting to use any geometric data, it is essential to ensure that the data have been computed, by calling the member function update() with arguments specifying exactly which geometric data are needed. For example, if the GenericGrid is actually a MappedGrid and some geometric data are needed which are defined in class MappedGrid, then update() must be called with arguments specifying which MappedGrid geometric data are needed. If the grid is changed in any way that could affect its geometric data, then these data are automatically marked out-of-date. The data are never recomputed until this is explicitly requested by a call to update(), with the arguments specifying exactly which geometric data are needed. This argument is an integer mask formed by taking the "bitwise or" of constants defined in the class GenericGrid and any class derived from it. These member functions may be used for any class derived from GenericGrid, such as class MappedGrid. Example 2.2 illustrates the use of these member functions. First, we find out which geometric data already have been computed. This information is returned by computedGeometry () as a mask of bits, where each bit refers to geometric data that are specific to the derived class of the grid. We store this mask in the integer cg. Next, we mark this geometric data out-of-date using geometryHasChanged(), as we might want to do if we had modified the grid in a way that would affect its geometric data. For example, if the grid was a MappedGrid and we had applied a rotation to its mapping, then all of the geometric data would become invalid and would need to be recomputed. Next, we destroy this geometric data using destroy(). We would not normally do this; we do it here only to show how it may be done. This reduces the storage used for the GenericGrid to the least possible. Finally, we recompute the geometric data specified by the mask cg.

```
#include "GenericGrid.h"
void example(GenericGrid g)
{
    Integer cg = g.computedGeometry(); // Check which geometric data are up-to-date.
    g.geometryHasChanged(cg); // Mark this geometric data out-of-date.
    g.destroy(cg); // Deallocate storage for this geometric data.
    g.update(cg); // Reallocate storage and compute this geometric data.
```

\}

Example 2.2: GenericGrid geometry management

### 2.3 Input/output and miscellaneous member functions

We list here some member functions of class GenericGrid for input/output of data structures, and any other member functions not mentioned above. Typically these member functions are overloaded in derived classes, and most of these are virtual member functions. The virtual member function initialize() is used to put the GenericGrid back into the state it was in after it was first constructed. However, this function is not particularly useful, because if the grid belongs to a derived grid class (as it usually does), it may have undesired side effects that leave the grid in a
state that is not self-consistent. Other examples are the member functions get() and put(), for reading and writing a GenericGrid to or from a database. An example of an overloaded function which is not a virtual function (and not even a member function) is the stream output operator. This function prints out a summary of the data of a GenericGrid. Example 2.3 illustrates the use of these functions.

```
#include "GenericGrid.h"
void example(GenericDataBase & file)
{
    GenericGrid g;
    g.get(file, "grid1"); // Read a GenericGrid named "grid1" from the file.
    g.put(file, "grid2"); // Write the GenericGrid to the file with name "grid2."
    cout << "g = " << endl << g << endl; // Print out the contents of g.
}
```

Example 2.3: Input/output of GenericGrids

## 3 Class MappedGrid

Class MappedGrid is used for all logically-rectangular grids. This includes cartesian, rectangular and curvilinear grids in one, two and three dimensions. Class MappedGrid allows for grids with holes, unused vertices or cells within a grid. It is assumed that a continuous function exists which maps the vertices of a uniform grid to the vertices of the MappedGrid. This is no restriction, becauase it is always possible to construct an interpolant function with this property. MappedGrid is derived from class GenericGrid (§2). It overloads some of the GenericGrid public constants, member data and member functions described in (§2). All of the member functions of class GenericGrid described there may be used; only note that now the copy constructor and the member functions reference() and operator $=()$ take a MappedGrid as their argument. There is an additional constructor for MappedGrid, which takes a Mapping as argument, as shown in Example 3.1. Corresponding to this constructor, there is also a reference() function which takes a Mapping as argument.

### 3.1 Geometry management

Class MappedGrid provides access to geometric data at the grid vertices. In addition, it provides access to geometric data at cell centers and other locations, as well as some global geometric data. However, to start the discussion, we consider first only the the global geometric data and the geometric data that class MappedGrid provides at the grid vertices. In particular, it provides access to the coordinates of the vertices as computed from the mapping, the derivative, the inverse derivative and the jacobian determinant of the derivative of the mapping at the vertices, as well as the unit outward normal vector at the boundary vertices of the grid. The global information it provides is a bounding box for vertices of the grid and, for each direction in the parameter space of the grid, the minimum and maximum distance between adjacent grid vertices. The grid vertices and other local geometric data computed at the grid vertices are stored in RealMappedGridFunctions, which are derived from $\mathbf{A}++$ arrays. The first three indices of these arrays indicate the particular grid vertex. The fourth index refers, in the case of the vertex coordinates, the mapping derivative and the normal vector, to the coordinate $(x, y, z)$; for the inverse mapping derivative it refers to the coordinate $\left(r_{1}, r_{2}, r_{3}\right)$. The fifth index refers, in the case of the mapping derivative, to the partial derivative $\left(\partial / \partial r_{1}, \partial / \partial r_{2}, \partial / \partial r_{3}\right)$; in the case of the inverse mapping derivative it refers to the partial derivative $(\partial / \partial x, \partial / \partial y, \partial / \partial z)$. For example, if the mapping is $\mathbf{d}:[0,1]^{3} \mapsto \mathbb{R}^{3}$ then
the coordinates of grid vertex $\left(i_{1}, i_{2}, i_{3}\right)$ are

$$
\mathbf{d}\left(r_{1}, r_{2}, r_{3}\right)=\left[\begin{array}{l}
x \\
y \\
z
\end{array}\right]_{i_{1}, i_{2}, i_{3}}=\left[\begin{array}{c}
\operatorname{vertex}\left(i_{1}, i_{2}, i_{3}, 0\right) \\
\operatorname{vertex}\left(i_{1}, i_{2}, i_{3}, 1\right) \\
\operatorname{vertex}\left(i_{1}, i_{2}, i_{3}, 2\right)
\end{array}\right]
$$

and the mapping derivative at grid vertex $\left(i_{1}, i_{2}, i_{3}\right)$ is

$$
\begin{aligned}
\frac{\partial \mathbf{d}}{\partial \mathbf{r}}\left(r_{1}, r_{2}, r_{3}\right) & =\left[\begin{array}{lll}
\frac{\partial x}{\partial r_{1}} & \frac{\partial x}{\partial r_{2}} & \frac{\partial x}{\partial r_{3}} \\
\frac{\partial y}{\partial r_{1}} & \frac{\partial y}{\partial r_{2}} & \frac{\partial y}{\partial r_{3}} \\
\frac{\partial z}{\partial r_{1}} & \frac{\partial z}{\partial r_{2}} & \frac{\partial z}{\partial r_{3}}
\end{array}\right]_{i_{1}, i_{2}, i_{3}} \\
& =\left[\begin{array}{llll}
\text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 0,0\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 0,1\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 0,2\right) \\
\text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 1,0\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 1,1\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 1,2\right) \\
\text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 2,0\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 2,1\right) & \text { vertexDerivative }\left(i_{1}, i_{2}, i_{3}, 2,2\right)
\end{array}\right] .
\end{aligned}
$$

The ranges of indices of grid vertices that lie in the interior or on the boundary of the grid are returned by the function gridIndexRange $(i, j)$, where $i=0$ refers to the lower bound for the index and $i=1$ refers to the upper bound; $j=0,1,2$ refers to the first, second or third index of the grid vertex. The geometric data are computed at grid vertices with indices in the range given by dimension $(i, j)$, which determines the array dimensions of the RealMappedGridFunctions, and may extend outside the boundary of the grid. Access to vertex data is shown in Example 3.1.

```
#include "MappedGrid.h"
#include "Annulus.h"
int
main()
{
    AnnulusMapping map;
    MappedGrid g = map; // Construct MappedGrid from a Mapping
    g.update(MappedGrid::THEvertex | // Update the grid vertex coordinates, the
        MappedGrid::THEvertexDerivative | // derivative of the mapping at the vertices,
        MappedGrid::THEinverseVertexDerivative | // the inverse derivative at the vertices, the
        MappedGrid::THEvertexJacobian | // jacobian determinant of the derivative, the
        MappedGrid::THEvertexBoundaryNormal | // unit outward normal at boundary vertices,
        MappedGrid::THEboundingBox | // the bounding box for grid vertices, and the
        MappedGrid::THEminMaxEdgeLength); // min.~and max. ~distance between vertices.
    RealMappedGridFunction & vertex = g.vertex(), // Access the grid vertices and the
        & vertexDerivative = g.vertexDerivative(); // mapping derivative at the grid vertices.
    Range dO = g.numberOfDimensions(), // The indices of the vertices corresponding
        I1(g.gridIndexRange (0,0),g.gridIndexRange(1,0)), // to interior and boundaries of the grid are
        I2(g.gridIndexRange(0,1),g.gridIndexRange(1,1)), // given by g.gridIndexRange. The
        I3(g.gridIndexRange(0,2),g.gridIndexRange(1,2)); // fourth index selects the (x,y,z) component.
    RealArray v;
    v = vertex(I1,I2,I3,d0); // Copy the grid vertices
    v.display("vertices");
    return 0;
}
```

Example 3.1: Access to MappedGrid grid vertex data
The data are computed and stored only when this is requested through a call to the update() member function with arguments specifying exactly which geometric data are needed. The "bitwise or" operator is used to combine several requests into one. The geometric data requested through the call to update() are computed only if it is determined that they are out-of-date. This would occur on the first call to update(), for example, or any time that the mapping is changed or the number of grid vertices is changed. (Note, however, that the MappedGrid is not able to determine if or when the user changes its mapping; in that case the user is responsible to call geometryHasChanged(), as explained in §2.2.) If update() were called again right away with the same arguments then no geometric data would be recomputed, because the data would already be marked up-to-date as a result of the previous call to update(). It is essential that update() be called in any function where geometric data are used, to update the specific geometric data needed in that function, if there is any possibility that the data may be out-of-date when the function is called. This is always safe to do and is never wasteful, because the only data recomputed are those which are still out-of-date.

The grid vertex data are used for graphics applications such as drawing a representation of the grid. They also could be used in the discretization of partial differential equations. However, we discourage their use in the discretization of PDEs. For this purpose, MappedGrid provides and we recommend instead the use of geometric data at points that we refer to as "discretization-cell centers," "discretization points," or simply "gridpoints." These are points where the discretization of a PDE is centered. For a vertex-centered discretization, as commonly used in finite-difference methods, the discretization points are identical to the grid vertices. For a cell-centered discretization, as commonly used in finite-volume methods, the discretization cells are grid cells, whose corners are the grid vertices.


Figure 1: Some MappedGrid centering options

These two options for grid centering are illustrated in Figure 1. The MappedGrid contains the notion of how it is centered. This is given by the member function isCellCentered $(i)$, which refers to the location of discretization points with respect to cells bounded by the grid vertices. For example, isCellCentered $(i)=$ LogicalFalse for $i=0, \ldots$, numberOfDimensions() - 1 for a vertex-centered grid, used for a vertex-centered discretization, and isCellCentered $(i)=$ LogicalTrue for $i=0, \ldots$, numberOfDimensions ()$-1$ for a cell-centered grid. Sometimes it is convenient to have available a PDE discretization that may be applied either at grid vertices or at grid-cell centers. To make it easy to implement such a discretization, MappedGrid provides geometric data at discretization points, and on faces and at corner of cells that are centered at discretization points. For a cell-centered grid, these cells are identical to the cells with grid vertices at their corners. However, for a vertex-centered grid, the corners of these cells form a dual grid. Some of the geometric data available at the discretization points are center, the coordinates of the discretization points, centerDerivative, inverseCenterDerivative and centerJacobian, the derivative, inverse derivative and the jacobian determinant of the derivative of the mapping computed at the discretization points. Example 3.1 shows how to access these data.

```
#include "MappedGrid.h"
#include "Annulus.h"
int
main()
{
    AnnulusMapping map;
    MappedGrid g = map; // Construct MappedGrid from a Mapping
    g.update(MappedGrid::THEcenter | // Update the discretization points, the
        MappedGrid::THEcenterDerivative | // derivative of the mapping,
        MappedGrid::THEinverseCenterDerivative | // the inverse derivative, and the
        MappedGrid::THEcenterJacobian ); // jacobian determinant of the derivative
    RealMappedGridFunction & center = g.center(); // Access the discretization points
    center.display("center");
    return 0;
}
```

Example 3.1: Access to MappedGrid discretization-point data
To aid in the implementation of finite-volume discretizations, MappedGrid provides additional geometric data about the discretization cells. In particular, it provides faceNormal, the inward normal vector to the left, bottom and back faces of the cell, normalized to the area of the face. (This assumes a right-handed coordinate system; for a left-handed coordinate system these vectors are outward normals.) It provides faceArea, the area of the left, bottom and back faces of the cell. Of course, the corresponding data on the right, top and front faces of the cell are
available also, as these faces are the left, bottom and back faces of neighbouring cells. Class MappedGrid provides also cellVolume, centerNormal and center Area. The latter two refer to faces formed by cutting the cell through its center in each direction. Finally, on the boundary of the grid, it provides centerBoundaryNormal, the unit outward normal vector, and centerBoundaryTangent, unit vectors tangent to the faces of cells on the boundary. These tangent vectors are not necessarily orthogonal to each other, although each of them is orthogonal to the normal vector. Class MappedGrid also provides access to corner, the coordinates of corners of the discretization cells. In the case of a cell-centered grid, these are identical with the grid vertices, while in the case of a vertex-centered grid, these form a dual grid, as mentioned above. Example 3.1 shows how to access these data. Sometimes it is interesting to compute the geometric data not directly from the mapping, but instead by using appropriate finite differences and/or averaging of the coordinates of the discretization-cell corners. This is common when the finite-volume discretization is defined using a geometric construction. In order to force the geometry to be computed in this way, an optional second argument to update() may be passed the value MappedGrid::USEdifferenceApproximation, as shown in Example 3.1.

```
#include "MappedGrid.h"
#include "Annulus.h"
int
main()
{
    AnnulusMapping map;
    MappedGrid g = map; // Construct MappedGrid from a Mapping
    g.changeToAllCellCentered(); // Make this a cell-centered grid.
    g.update(MappedGrid::THEcorner | // Update the discretization cell corners,
        MappedGrid::THEfaceNormal | // the cell face normal vectors,
        MappedGrid::THEfaceArea | // the cell face areas,
        MappedGrid::THEcellVolume | // the cell volumes,
        MappedGrid::THEcenterNormal | // the cell-centered normal vectors,
        MappedGrid::THEcenterArea | // the cell-centered face areas,
        MappedGrid::THEcenterBoundaryNormal | // the unit normals to the grid boundaries, and
        MappedGrid::THEcenterBoundaryTangent | // the unit tangents to the grid boundaries.
        MappedGrid::USEdifferenceApproximation); // Compute the the cell corners from the mapping,
                                    // and compute everything else from the corners by
                                    // finite differences and averaging of corner data.
    RealMappedGridFunction & corner = g.corner(); // Access the discretization points
    corner.display("corner");
    return 0;
}
```

Example 3.1: Access to MappedGrid data used for finite-volume discretizations

### 3.2 Access to MappedGrid parameters

Class MappedGrid has many useful parameters that may accessed and modified in order to make the grid useful for the discretization of a given PDE problem. For example, as we mentioned above, a MappedGrid may be vertex-centered or cell-centered. There are parameters that may be modified by the user in order to change the grid from vertex-centered to cell-centered and vice versa. The parameters of a MappedGrid may be divided into several broad categories. First, there are parameters describing the dimensions of the index space of data (such as gridpoints) on the grid. Second, there are parameters describing the topology of the grid. Third, there are parameters describing discretization stencils used on the grid. The cell-centering is such a parameter. All of these parameters have reasonable default values; some of these are determined from the mapping that describes the grid. Many of these parameters may be set or changed by the user; the rest are recomputed whenever update() is called, in order to make all of the parameters consistent with each other. Whenever any of these parameters is changed, and the result of the change makes some of the geometric data invalid, the data that become invalid are marked out-of-date. For example, if the number of gridpoints is changed, then all geometric data that are computed on the gridpoints (such as the coordinates of the grid vertices) become invalid. It is the user's responsibility to call update() again with arguments that specify which geometric data are needed, in order to recompute geometric data that are still needed but have become out-of-date. For example, if center, the coordinates of the discretization points, is needed again after the number of gridpoints has changed, then it is necessary to call update() and pass MappedGrid::THEcenter as its argument. If this step is omitted, then center will either be empty, or it will
have the wrong dimensions, or it will contain incorrect data. There is no warning given when geometric data become out-of-date, because there is no assumption made about which data will be needed again unless and until update() is called to specify exactly which geometric data are still needed.

The MappedGrid parameters that describe the index space of grid data are indexRange, extendedIndexRange, gridIndexRange, dimension and numberOfGhostPoints. The parameters that may be set by the user are gridIndexRange and numberOfGhostPoints; the other parameters are automatically computed from these whenever update() is called. The parameter gridIndexRange gives the indices of grid vertices corresponding to each boundary of the grid. In the index space of the grid, where the grid vertices form an integer lattice, we refer to the left, right, bottom, top, back and front sides of the grid, where the first, second and third indices of grid vertices take their lower and upper bound, respectively. The lower and upper bounds of the first index of the grid vertices on the boundary are gridIndexRange ( 0,0 ) and gridIndexRange $(1,0)$, respectively; the lower and upper bounds of the second index are gridIndexRange $(0,1)$ and gridIndexRange $(1,1)$, and the lower and upper bounds of the third index are gridIndexRange $(0,2)$ and gridIndexRange $(1,2)$. These are initially determined from the mapping that describes the grid; the user may change them using the function setGridIndexRange(). The parameter numberOfGhostPoints gives the width of a band of extra gridpoints that lie outside the boundary of the grid. These extra gridpoints are not usually considered to be part of the grid, but may be convenient to have for the discretization of a PDE. There is no guarantee that the mapping is well-behaved at these points. The number of ghost points on the left and right sides of the grid are given by numberOfGhostPoints $(0,0)$ and numberOfGhostPoints $(1,0)$, respectively; on the bottom and top, numberOfGhostPoints $(0,1)$ and numberOfGhostPoints $(1,1)$; and on the back and front, numberOfGhostPoints $(0,2)$ and numberOfGhostPoints $(1,2)$. These are initially set to one, which may be convenient for a discretization-stencil width of three. They may be set using the function setNumberOfGhostPoints(). All of the other parameters that describe the index space of grid data are recomputed whenever update () is called. For example, dimension, the dimensions used for the arrays of grid data, is set to gridIndexRange plus or minus numberOfGhostPoints. The parameter indexRange gives the lower and upper bounds for the discretization points in the interior and on the boundary of the grid. For a vertex-centered grid, indexRange is identical to gridIndexRange, because the discretization points are the grid vertices. The exception to this rule is a periodic grid, in which case the first and last gridpoints are equivalent; the last gridpoint is considered redundant for the purposes of discretization, so it is not included in the range of discretization points, and indexRange $(1, i)=$ gridIndexRange $(1, i)-1$ in the periodic direction $i$. For a cell-centered grid, the discretization points are grid-cell centers. In each direction the number of cells is one fewer than the number of grid vertices. The cell centers are numbered the in same way as their lower-left corners (i.e., the grid vertices), so indexRange $(0, i)=\operatorname{gridIndexRange}(0, i)$ and indexRange $(1, i)=\operatorname{gridIndexRange}(1, i)-1$ on a cell-centered grid. To summarize, indexRange is the same as gridIndexRange, except in directions where the grid is either periodic or cell-centered, in which cases the upper bound indexRange $(1, i)$ is less by one. The parameter extendedIndexRange is identical to indexRange with the possible exception that on sides of the grid where there is no boundary condition specified, extendedIndexRange may include a strip of ghost points as wide as (discretizationWidth -1$) / 2$. This strip of ghost points is included only if the flag useGhostPoints() is set to LogicalTrue. By default, this flag is set to LogicalFalse; it may be changed by calling the function setUseGhostPoints(). Example 3.2 shows how to access and set the parameters that describe the index space of grid data.

```
```

\#include "MappedGrid.h"

```
```

\#include "MappedGrid.h"
\#include "Annulus.h"
\#include "Annulus.h"
int
int
main()
main()
{
{
AnnulusMapping map;
AnnulusMapping map;
MappedGrid g = map;
MappedGrid g = map;
printf("gridIndexRange=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the range of indices for grid vertices.
printf("gridIndexRange=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the range of indices for grid vertices.
g.gridIndexRange (0,0),g.gridIndexRange(1,0),
g.gridIndexRange (0,0),g.gridIndexRange(1,0),
g.gridIndexRange(0,1),g.gridIndexRange(1,1),
g.gridIndexRange(0,1),g.gridIndexRange(1,1),
g.gridIndexRange(0,2),g.gridIndexRange(1,2));
g.gridIndexRange(0,2),g.gridIndexRange(1,2));
printf("indexRange=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the range for discretization points.
printf("indexRange=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the range for discretization points.
g.indexRange ( 0,0),g.indexRange (1,0),
g.indexRange ( 0,0),g.indexRange (1,0),
g.indexRange (0,1),g.indexRange (1,1),
g.indexRange (0,1),g.indexRange (1,1),
g.indexRange (0,2),g.indexRange (1,2));

```
```

        g.indexRange (0,2),g.indexRange (1,2));
    ```
```

```
    printf("numberOfGhostPoints=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the number of ghost points
            g.numberOfGhostPoints ( 0,0),g.numberOfGhostPoints(1,0),
            g.numberOfGhostPoints(0,1),g.numberOfGhostPoints(1,1),
            g.numberOfGhostPoints(0,2),g.numberOfGhostPoints(1,2));
    printf("dimension=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the grid dimensions
            g.dimension(0,0),g.dimension(1,0),
            g.dimension(0,1),g.dimension(1,1),
            g.dimension(0,2),g.dimension(1,2));
    int axis;
    for( axis=0; axis<g.numberOfDimensions(); axis++ )
    {
        g.setIsCellCentered(axis,LogicalTrue); // Change the grid to cell-centered
        g.setNumberOfGhostPoints(0,axis, 2); // Change the number of ghost points on the left side
        g.setNumberOfGhostPoints(1,axis, 2); // Change the number of ghost points on the right side
    }
    g.update(MappedGrid::THEvertex); // Compute the geometry;
    return 0;
```

\}

```
gridIndexRange = [0,20]x[0,6]x[0,0]
indexRange=[0,19]x[0,6]x[0,0]
numberOfGhostPoints=[1,1]x[1,1]x[0,0]
dimension=[-1,21]x[-1,7]x[0,0]
```

Example 3.2: Access to MappedGrid index-space data
The MappedGrid parameters that describe the topology of the grid are numberOfDimensions, isPeriodic, boundaryCondition, sharedBoundaryFlag and sharedBoundaryTolerance. All of these parameters have default values determined from the mapping that describes the grid. These parameters may all be set by the user. However, it is important that they be set in such a way as to be consistent with the mapping. At this time I can think of no good reason to change numberOfDimensions; to do so would probably cause all kinds of trouble. Its initial value is that of the Mapping member function getRangeDimension(), which we assume is equal to getDomainDimension(). The parameter isPeriodic gives the periodicity of the grid in each coordinate direction. If the grid itself is periodic, then isPeriodic should be set to Mapping::functionPeriodic; otherwise, if the PDE problem to be solved on the grid is periodic, then isPeriodic should be set to Mapping::derivativePeriodic; otherwise isPeriodic should be set to Mapping::notPeriodic. The parameter boundaryCondition should be positive on each side of the grid that corresponds to a domain boundary. It should be negative on both opposite sides of the grid in each direction where either the domain is periodic or the PDE problem to be solved on the grid is periodic. In any case, the parameters boundaryCondition and isPeriodic must be set so that they are consistent with each other. The parameters sharedBoundaryFlag and sharedBoundaryTolerance are useful only in situations where several MappedGrids overlap to cover the domain. Class CompositeGrid contains MappedGrids used for this purpose, so the discussion of these parameters is deferred. The use of the MappedGrid parameters that describe the topology of the grid is shown in Example 3.2.

```
#include "MappedGrid.h"
#include "Annulus.h"
int
main()
{
    AnnulusMapping map;
    MappedGrid g = map;
    printf("isPeriodic=[%i,%i,%i]\n", // Print out the periodicity of each grid coordinate
        g.isPeriodic(axis1),g.isPeriodic(axis2),g.isPeriodic(axis3));
    printf("boundaryCondition=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the boundary condition for each side.
```

```
        g.boundaryCondition(0,0),g.boundaryCondition(1,0),
        g.boundaryCondition(0,1),g.boundaryCondition(1,1),
        g.boundaryCondition(0,2),g.boundaryCondition(1,2));
    printf("numberOfGhostPoints=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print out the shared boundary flag.
        g.sharedBoundaryFlag(0,0),g.sharedBoundaryFlag(1,0),
        g.sharedBoundaryFlag(0,1),g.sharedBoundaryFlag(1,1),
        g.sharedBoundaryFlag(0,2),g.sharedBoundaryFlag(1,2));
    printf("sharedBoundaryTolerance=[%f,%f]x[%f,%f]x[%f,%f]\n", // Print out the shared boundary tolerance
        g.sharedBoundaryTolerance (0,0),g.sharedBoundaryTolerance(1,0),
        g.sharedBoundaryTolerance(0,1),g.sharedBoundaryTolerance(1,1),
        g.sharedBoundaryTolerance(0,2),g.sharedBoundaryTolerance(1,2));
    g.setIsPeriodic(axis1,Mapping::notPeriodic); // Make the grid not periodic
    g.setBoundaryCondition(0,axis1, 2); // assign boundary condition values.
    g.setBoundaryCondition(1,axis1, 3);
    g.update(MappedGrid::THEvertex);
    return 0;
}
```

isPeriodic=[2, 0,1]
boundaryCondition $=[-1,-1] \times[1,2] \times[-1,-1]$
numberOfGhostPoints $=[0,0] x[0,0] x[0,0]$
sharedBoundaryTolerance $=[0.100000,0.100000] \times[0.100000,0.100000] \times[0.000000,0.000000]$

Example 3.2: Access to MappedGrid topology data
The MappedGrid parameters that describe discretization stencils used on the grid are discretizationWidth, boundaryDiscretizationWidth, isCellCentered, isAllCellCentered, isAllVertexCentered and gridSpacing. All of these have default values. The parameters discretizationWidth, boundaryDiscretizationWidth and isCellCentered may be set by the user; the others are automatically computed whenever update() is called. The parameter discretizationWidth refers to the width of the interior discretization stencil in each coordinate direction, and may be set to any positive odd integer. (A centered discretization is assumed.) The default value for discretizationWidth is three. The parameter boundaryDiscretizationWidth refers to the width, in the normal direction, of the discretization stencil of the boundary conditions on each side of the grid. This width does not include any ghost points that may or may not be used in the discretization of the boundary conditions. The stencil width in the tangential directions is assumed to be equal to the interior discretization-stencil width in those directions. This width may be any positive integer. The default value for boundaryDiscretizationWidth is three, which is convenient for a second-order one-sided approximation to the normal derivative. The parameter isCellCentered refers to the centering of discretization points within the cells of the grid. By default, isCellCentered $(i)$ is LogicalFalse in each direction $i$, to indicate a vertex-centered grid. The parameter isCellCentered $(i)$ may be set independently for each direction $i$, so that face-centered and edge-centered grids are possible in addition to vertex-centered and cell-centered grids. However, I can think of no possible use for a face-centered or edge-centered grid. Certainly some geometrical data such as face normal vectors may be face-centered, but this has nothing to do with whether or not the grid itself is face-centered. The parameter isAllCellCentered is computed by update() and is LogicalTrue only if isCellCentered $(i)$ is LogicalTrue for all directions $0<i<$ numberOfDimensions(). Likewise, the parameter isAllVertexCentered is computed by update() and is LogicalTrue only if isCellCentered $(i)$ is LogicalFalse for all directions $0<i<$ numberOfDimensions(). Finally, the parameter discretizationWidth is computed by update() to be the distance between gridpoints on the uniform rectangular grid on the unit-square parameter space of the grid and its mapping. The use of the MappedGrid parameters that describe discretization stencils on the grid is shown in Example 3.2.

```
#include "MappedGrid.h"
#include "Annulus.h"
int
main()
{
    AnnulusMapping map;
```

```
    MappedGrid g = map;
    printf("discretizationWidth=[%i,%i,%i]\n", // Print out the interior discretization width
            g.discretizationWidth(axis1),g.discretizationWidth(axis2),g.discretizationWidth(axis3));
    printf("boundaryDiscretizationWidth=[%i,%i]x[%i,%i]x[%i,%i]\n", // Print boundary discretization width
        g.boundaryDiscretizationWidth(0,0),g.boundaryDiscretizationWidth(1,0),
        g.boundaryDiscretizationWidth(0,1),g.boundaryDiscretizationWidth(1,1),
        g.boundaryDiscretizationWidth(0,2),g.boundaryDiscretizationWidth(1,2));
    printf("gridSpacing=[%f,%f,%f]\n", // Print out the unit square spacing in each direction
        g.gridSpacing(axis1),g.gridSpacing(axis2),g.gridSpacing(axis3));
    printf("isCellCentered=[%i,%i,%i]\n", // Print te cell-centering in each direction.
            g.isCellCentered(axis1),g.isCellCentered(axis2),g.isCellCentered(axis3));
    printf("isAllCellCentered=%i\n",g.isAllCellCentered()); // Print out the cell-centering of the grid
    printf("isAllVertexCentered=%i\n",g.isAllVertexCentered());
    int axis;
    for( axis=0; axis<g.numberOfDimensions(); axis++ )
        g.setIsCellCentered(axis,LogicalTrue); // Change the grid to cell-centered
    g.update(MappedGrid::THEvertex);
    return 0;
```

\}

```
discretizationWidth=[3,3,1]
boundaryDiscretizationWidth=[3,3]x[3,3]x[1,1]
gridSpacing=[0.050000,0.166667,1.000000]
isCellCentered=[0,0,0]
isAllCellCentered=0
isAllVertexCentered=1
```

Example 3.2: Access to MappedGrid discretization-stencil data
There are two exceptions to the rule that geometric data invalidated by changes to parameters are not automatically updated at the same time as the parameter changes are made. The member functions changeToAllCellCentered() and changeToAllVertexCentered() cause any geometric data that were up-to-date before the call to be recomputed if the parameter changes caused them to become invalid. This is supposed to be useful in the case where the only parameter changes needed are to change the grid either to cell-centered or to vertex-centered. If any other parameters need to be changed also, then the geometric data may become invalid as a result of these other changes, and it would be a waste of time to have these member functions recompute the geometric data before all of the changes have been made. Also, it is wasteful to update the geometric data before changing the grid to cell-centered or vertex-centered, as some of the geometric data will usually need to be recomputed. Clearly, these member functions should be used with care if they are used at all.

### 3.3 Miscellaneous member functions

Class MappedGrid has a few member functions not mentioned above. These functions are probably not needed by most people. The function box() returns a reference to a Boxlib Box object that contains index-space and cellcentering information about the MappedGrid. This information is redundant in the sense that it duplicates the information returned by indexRange() and isCellCentered(). However, it may be useful for interfacing with code that uses Boxlib. The function adjustBoundary () is used to force the parameter-space coordinates ( $r_{1}, r_{2}, r_{3}$ ) of a point to zero or one, as appropriate, if the point is on a boundary of another grid that is shared with the corresponding boundary of this grid. The function getInverseCondition() computes a condition number for the sensitivity of the parameter-space coordinates $\left(r_{1}, r_{2}, r_{3}\right)$ in this grid of a point from another grid, to errors in the coordinates of the point in the parameter space of the other grid. This condition number is used in estimates of the truncation error for interpolation of data from the other grid. The function specifyProcesses() is used to specify how data (such
as geometric data) on the MappedGrid are distributed over processes on a multiprocessor computer. The function initialize() is used to put the MappedGrid back into the state it was in after it was first constructed, supposing that it was constructed using its current mapping. In this state, the geometric data are marked out-of-date and their storage is dellocated. This function should be used with care, because if the grid belongs to a derived grid class, it may have undesired side effects that leave the grid in a state that is not self-consistent. In addition to these functions, the member functions of the base grid class GenericGrid are accessible from MappedGrid, either directly as they are described in $\S 2$ or as overloaded functions defined in class MappedGrid.

## 4 Class GenericGridCollection

Class GenericGridCollection is the base class for all Overture classes that contain collections of grids. It is derived from class ReferenceCounting (Appendix A), just as class GenericGrid is. As a consequence, the entire discussion of data-sharing in $\S 2.1$ and Example 2.1 applies directly to class GenericGridCollection. For each GenericGrid member function discussed there, there is a corresponding GenericGridCollection member function. The only difference is that the default constructor and member function initialize() take an optional argument specifying the number of grids initially in the collection, as shown in Example 4.1. The discussion of geometry management in $\S 2.2$ and Example 2.2 also applies directly to class GenericGridCollection. Whenever the GenericGridCollection member functions update(), destroy (), or geometryHasChanged() are called, these in turn call the corresponding function for each grid in the collection, passing on the arguments that specify the geometric data. In addition, these member functions are used to manage the geometric data discussed in $\S 4.1$, as shown in Example 4.1. The discussion of the miscellaneous functions in $\S 2.3$ and Example 2.3 also applies directly to class GenericGridCollection. It is a valuable exercise to review $\S 2$ in its entirety, mentally substituting GenericGridCollection everywhere that GenericGrid appears there.


The domain



Two base grids covering the domain

Figure 2: A computational domain covered by a GenericGridCollection of two base grids. The cross-hatch patterns abstractly represent the base grids. However, since the grids are only GenericGrids, which have no particular structure, these patterns are are not intended to imply the structure of the grids. The grids may be rectangular, unstructured triangular, or who knows what else.

Class GenericGridCollection contains a collection of GenericGrids that may be indexed using the member function operator[](), and it may be used as merely a collection of grids. However, it provides a mechanism for adding some structure to this collection. Each grid added to the collection is called a "base grid," to indicate that these grids are independent of and unrelated to each other. A base grid may cover the entire domain of the problem under consideration, or it may possibly cover only part of the domain, in which case we expect to have several base grids which together cover the entire domain. If there is more than one base grid, then each of the base grids is normally expected to cover a different part of the domain, although possibly with some overlap. It is expected that all of the base grids are needed in order to describe the domain accurately, and that if any of the base grids were omitted then the description of the domain would be incomplete or at best inaccurate. Figure 2 shows a cartoon of a domain covered by two base grids. The structure of the base grids is intended to be ambiguous, since these are GenericGrids
and therefore have no particular structure. In a concrete example, these grids would belong to a derived grid class and would have some geometric structure. For example, the base grids might be MappedGrids, in which case they would have logically-rectangular geometric structure that includes curvilinear gridlines, quadrilateral or hexahedral cells, and the like. This figure is supposed to convey the concept of a GenericGridCollection consisting of two base grids that do not overlap but which together cover the domain completely. Example 4.1 shows how a GenericGridCollection may be constructed with two grids that are also two base grids.

### 4.1 Local refinements and multigrid coarsenings



Two base grids


Base grids with one refinement each

Figure 3: Some GenericGridCollection base grids and local refinements. Each base grid has one level-one refinement grid. This GenericGridCollection has two base grids and two refinement levels.

Corresponding to each base grid in a GenericGridCollection, there may also be some local refinement grids. All of the refinements of a base grid are related to that base grid, in the sense that they each cover either the same sub-domain as that of the unrefined base grid, or perhaps only a part of that sub-domain. In other words, each refinement grid is a refinement of only one base grid, and does not cover any part of the domain which is not already covered by that base grid. Each base grid and refinement grid is labeled by a base grid number and a refinement level number. Each unrefined base grid has a unique base grid number and has refinement level number zero; its refinements have the same base grid number and have refinement level number one. The union of the level-one refinements of an unrefined base grid covers a sub-domain within that of the base grid. If this sub-domain is refined further, then these further refinements have refinement level number two. In this way an arbitrary number of nested refinement levels may be added to a base grid, each consisting of one or more local refinement grids. In other words, the refinement levels form successively finer representations of nested sub-domains. If the GenericGridCollection contains more than one base grid, then the collection of grids may be partitioned into disjoint subsets of grids that belong to each of the unrefined base grids (those grids which have in common their base grid number). Class GenericGridCollection contains a collection of GenericGridCollections that hold the subsets of grids that form this partition. It also contains a collection of GenericGridCollections that hold the disjoint subsets of grids that have in common their refinement level number, without consideration of which base grids they refine. Each of these subsets may contain refinements of more than one base grid, if it happens that different base grids each have refinements at the same refinement level. The two partitions of the collection of grids into subsets according to their base grid number and according to their refinement level number are arthogonal to each other in the sense that these two partitioning criteria are independent of each other. Figure 3 shows on the left a domain covered by two base grids; on the right it shows these base grids each partially covered by a level-one local refinement grid. Example 4.1 shows how a refinement may be added to each of two base grids, so that afterward the GenericGridCollection has two refinement levels and two base grids, each with one level-one refinement, for a total of four grids.

Each base grid or refinement grid in a GenericGridCollection may be coarsened for the purposes of multigrid, and may have several levels of multigrid coarsening. Each base grid or refinement grid, before coarsening for multigrid, is called a "component grid." Each multigrid coarsening covers the same subdomain as the component grid that it


Two component grids (base grids)


One coarsening of each component grid

Figure 4: Some GenericGridCollection component grids and multigrid coarsenings. The component grids in this case are base grids. Each component grid has one level-one multigrid coarsening. This GenericGridCollection has two component grids and two multigrid levels.
coarsens. If there is more than one level of multigrid coarsening, then each multigrid level is a coarsening of the grid that forms the preceding multigrid level. In other words, the multigrid levels form successively coarser representations of the sub-domain covered by their corresponding component grid (which may itself be either a base grid or a refinement grid). Each component grid and multigrid coarsening is labeled with a component grid number and a multigrid level number. Each component grid has a unique component grid number and has multigrid level number zero; its multigrid coarsenings have the same component grid number and have increasing multigrid level numbers according to the number of times they have been coarsened. If there is more than one component grid, the collection of grids may be partitioned into disjoint subsets of grids that have the same component grid number. Class GenericGridCollection contains a collection of GenericGridCollections that hold the subsets of grids that form this partition. It also contains a collection of GenericGridCollections that holds the disjoint subsets of grids that have in common their multigrid level number. The two partitions of the collection of grids into subsets according to their component grid number and according to their multigrid level number are arthogonal to each other in the sense that these two partitioning criteria are independent of each other. Figure 4 shows on the left a domain covered by two base grids, each of which is a component grid; on the right it shows level-one multigrid coarsenings of these component grids. Example 4.1 shows how a multigrid coarsenings may be added to each of four component grids, two of which are base grids and two are refinements, so that afterward the GenericGridCollection has two base grids at two refinement levels, for a total of four component grids, and each of these has three multigrid levels, for a total twelve grids.

```
#include "GenericGridCollection.h"
void
print(GenericGridCollection & gc)
{
    printf("numberOfGrids=%i, numberOfBaseGrids=%i, numberOfComponentGrids=%i\n"
        "numberOfRefinementLevels=%i, numberOfMultigridLevels=%i\n",
        gc.numberOfGrids(),gc.numberOfBaseGrids(),gc.numberOfComponentGrids(),
        gc.numberOfRefinementLevels(),gc.numberOfMultigridLevels());
}
int
main()
{
    GenericGridCollection gc(2); // GenericGridCollectionwith 2 base grids
    printf("Initial:\n"); print(gc);
```

```
    int grid;
    for( grid=0; grid<gc.numberOfBaseGrids(); grid++ )
        gc.addRefinement(1,grid);
    printf("After add refinement:\n"); print(gc);
    int level;
    for( level=1; level<3; level++ )
        for( grid=0; grid<gc.numberOfComponentGrids(); grid++ )
            gc.addMultigridCoarsening(level,grid);
    printf("After add multigrid coarsenings:\n"); print(gc);
    gc.update(GenericGridCollection::THEbaseGrid); // Partition g according to base grid number.
    GenericGridCollection & gc1=gc.baseGrid[1]; // Access base grid one and its refinements.
    gc1.update(GenericGridCollection::THEmultigridLevel); // Partition g1 according to multigrid level.
    GenericGridCollection & gc12=gc1.multigridLevel[2]; // Access base grid one and its refinements
                                    // at multigrid level two.
    return 0;
```

\}

```
Initial:
numberOfGrids=2, numberOfBaseGrids=2, numberOfComponentGrids=2
numberOfRefinementLevels=1, numberOfMultigridLevels=1
After add refinement:
numberOfGrids=4, numberOfBaseGrids=2, numberOfComponentGrids=4
numberOfRefinementLevels=2, numberOfMultigridLevels=1
After add multigrid coarsenings:
numberOfGrids=12, numberOfBaseGrids=2, numberOfComponentGrids=4
numberOfRefinementLevels=2, numberOfMultigridLevels=3
```

Example 4.1: Access to partitions of a GenericGridCollection
To summarize, the collection of grids in a GenericGridCollection may be partitioned according to base grid or refinement level, and these two partitions are orthogonal to each other. Similarly, the collection may be partitioned according to component grid or multigrid level, and these two partitions also are orthogonal to each other. Since the collections forming the subsets in any of these four partitions are also GenericGridCollections, they may be further partitioned in exactly the same ways. For example, it is possible in this way to form a collection of all the refinements of a particular base grid at a given multigrid level. Example 4.1 shows how member functions update() and operator[]() may be used to partition a GenericGridCollection in this way.

### 4.2 Miscellaneous member functions

We describe here some member functions of class GenericGridCollection that were not mentioned above. Typically these member functions are overloaded in derived classes, and most of these are virtual member functions. The virtual member functions deleteMultigridCoarsening() and deleteMultigridLevels() are used to delete multigrid coarsenings. The latter deletes all coarsenings whose multigrid levels are higher than the level specified. Similarly, member functions deleteRefinement() and deleteRefinementLevels() are used to delete refinement grids; the latter deletes all refinement grids whose refinement levels are higher than the level specified. Sometimes it is useful and efficient to be able to have a "new" GenericGridCollection that shares all of the unrefined grids of an "old" GenericGridCollection. A different set of refinements may be added to the new collection so that it becomes appropriately adapted to new data. At this point, the old and new GenericGridCollections share the same base grids but have distinct sets of refinements. The virtual member function referenceRefinementLevels() provides this capability. It causes one GenericGridCollection to share with another GenericGridCollection all grids with refinement levels up to a given level of refinement. In order to share only the base grids, you would
pass arguments to specify level zero. The member function getIndex () is used to look for a GenericGrid within a GenericGridCollection. It returns the index of the grid within the collection, if the grid is found; otherwise it returns a negative number to indicate that the grid was not found. The GenericGrid member functions operator $==()$ and operator $!=()$ are used in this search. Example 4.2 shows how some of these member functions may be used.

```
#include "GenericGridCollection.h"
void
print(GenericGridCollection & gc)
{
    printf("numberOfGrids=%i, numberOfBaseGrids=%i, numberOfComponentGrids=%i\n"
        "numberOfRefinementLevels=%i, numberOfMultigridLevels=%i\n",
        gc.numberOfGrids(),gc.numberOfBaseGrids(),gc.numberOfComponentGrids(),
        gc.numberOfRefinementLevels(),gc.numberOfMultigridLevels());
    }
int
main()
{
    GenericGridCollection gc1(2), gc2;
    int grid,level;
    for( level=1; level<3; level++ )
        for( grid=0; grid<gc1.numberOfBaseGrids(); grid++ )
            gc1.addRefinement(level,grid); // Add level-one and level-two refinements of each base grid.
    for( level=1; level<3; level++ )
        for( grid=0; grid<gc1.numberOfComponentGrids(); grid++ ) // Add level-one and level-two multigrid
            gc1.addMultigridCoarsening(level,grid); // coarsenings of each component grid.
    printf("gc1 after adding grids:\n"); print(gc1);
    gc2.referenceRefinementLevels(gc1, 1); // Share grids with gc1 that have refinement level at most one.
    printf("gc2 after reference:\n"); print(gc2);
    gc1.deleteRefinementLevels(1); // Delete refinements with refinement levels higher than one.
    gc1.deleteMultigridLevels(1); // Delete coarsenings with multigrid levels higher than one.
    printf("gc1 after deleting grids:\n"); print(gc1);
    GenericGrid & g1 = gc1[0]; assert(gc1.getIndex (g1) == 0); // Check that g1 is in gc1 at index zero.
    GenericGrid g2; assert(gc1.getIndex(g2) < 0); // Check that g2 is not in gc1.
    return 0;
}
```

------------------------ output ----------------------------
gc1 after adding grids:
numberOfGrids=18, numberOfBaseGrids=2, numberOfComponentGrids=6
numberOfRefinementLevels=3, numberOfMultigridLevels=3
gc2 after reference:
numberOfGrids=12, numberOfBaseGrids=2, numberOfComponentGrids=4
numberOfRefinementLevels=2, numberOfMultigridLevels=3
gc1 after deleting grids:
numberOfGrids=8, numberOfBaseGrids=2, numberOfComponentGrids=4
numberOfRefinementLevels=2, numberOfMultigridLevels=2

Example 4.2: Miscellaneous GenericGridCollection member functions

## 5 Class GridCollection

Class GridCollection is the base class for all Overture classes that contain collections of MappedGrids. It is derived from class GenericGridCollection. It overloads some of the GenericGridCollection public constants, member data and member functions described in $\S 4$. All of the member functions of class GenericGridCollection described there may be used; only note that the default constructor and member function initialize() take an additional optional argument specifying the number of dimensions of the grids initially in the collection, and the copy constructor and the member functions reference() and operator=() now take a GridCollection as their argument. Also, the overloaded member functions addRefinement() and addMultigridCoarsening() take additional arguments that describe how the refinements and coarsenings are constructed from the corresponding lower refinementlevel or multigrid-level grids, as explained in $\S 5.1$. Class GridCollection has additional and member functions boundingBox, numberOfDimensions(), changeToAllVertexCentered() and changeToAllCellCentered() that correspond to the MappedGrid member functions of the same names. The member function boundingBox returns coordinate bounds of the smallest box containing the bounding boxes of all of the MappedGrids in the collection; this bounding box is computed by update(). The member function numberOfDimensions() returns the same value as the corresponding member functions of all of the MappedGrids in the collection (which must all agree). The member functions changeToAllVertexCentered() and changeToAllCellCentered() cause the corresponding member function to be called for each MappedGrid in the collection. Example 5 shows how some of these member functions may be used.

```
#include "Square.h"
#include "GridCollection.h"
int
main()
{
    GridCollection g(2,1); // Start with one two-dimensional grid.
    // GridCollection g; g.initialize(2,1); // This would have the same effect.
    int base = 0, ratio = 2, level = 1, refinement; // The base grid is grid zero.
    SquareMapping square(0.,1.,0.,1.); // A Mapping for the square [0,1]x[0,1].
    g[base].reference(square); // Make the base grid use the square mapping.
    g.update(GridCollection::THEboundingBox); // Update and print out the bounding box
    printf("boundingBox=[%f,%f]x[%f,%f]x[%f,%f]\n",
        g.boundingBox (0,0),g.boundingBox (1,0),
        g.boundingBox(0,1),g.boundingBox(1, 1),
        g.boundingBox(0,2),g.boundingBox(1,2));
    g.changeToAllVertexCentered(); // Make the base grid vertex-centered.
    IntegerArray range = g[base].indexRange(); // Find the index range of discretization points.
    range (0,0) = range (0,1) = 1; range (1,0) = range (1,1) = 3; // Refine the index range [1:3,1:3].
    refinement = g.addRefinement(range, ratio, level, base); // Add a level-one refinement grid.
    g.deleteRefinement(refinement); // Delete the refinement grid.
    g.changeToAllCellCentered(); // Make the base grid cell-centered.
    range = g[base].indexRange(); // Find the index range of discretization points.
    range(0,0) = range (0,1) = 1; range(1,0) = range(1,1) = 2; // Refine the index range [1:2,1:2].
    refinement = g.addRefinement(range, ratio, level, base); // Add a level-one refinement grid.
    g.deleteRefinement(refinement); // Delete the refinement grid.
    int component=0,coarsening;
    coarsening = g.addMultigridCoarsening(ratio, level, component); // Add a level-one multigrid coarsening.
    g.deleteMultigridCoarsening(coarsening); // Delete the multigrid coarsening.
    int grid;
    for( grid=0; grid<g.numberOfGrids(); grid++ )
    {
        printf("refinementFactor=[%i,%i,%i]\n", // Print the refinement factors
            g.refinementFactor(axis1),g.refinementFactor(axis2),g.refinementFactor(axis3));
        printf("multigridCoarseningFactor=[%i,%i,%i]\n", // Print the multigrid coarsening factors
```

```
g.multigridCoarseningFactor(axis1),g.multigridCoarseningFactor(axis2),
            g.multigridCoarseningFactor(axis3));
        printf("refinementFactor=[%i,%i,%i]\n", // Print the multigrid refinement factors
            g.refinementFactor(axis1),g.refinementFactor(axis2),g.refinementFactor(axis3));
        }
        return 0;
}
```

boundingBox $=[0.000000,1.000000] \times[0.000000,1.000000] \times[0.000000,0.000000]$
refinementFactor $=[1,1,1]$
multigridCoarseningFactor=[1,1,1]
refinementFactor=[1,1,1]

Example 5: Some GridCollection member functions

### 5.1 Local refinements and multigrid coarsenings




Cell-centered grid

Figure 5: Alignment of MappedGrid refinements for vertex-centered and for cell-centered grids. In this example, the refinement ratio in each direction is two. The range of indices of the base grid discretization points to be refined is indicated; for the vertex-centered case the range is $[1: 3,1: 3]$, while for the cell-centered case the range is $[1: 2,1: 2]$. The base-grid and refinement-grid vertices with indices zero are aligned, even though these vertices may lie outside the base grid or the refinement grid.

Class GridCollection contains a collection of MappedGrids. This is indexed using the overloaded member function operator[](). It also contains baseGrid, refinementLevel, componentGrid, and multigridLevel, collections of GridCollections that overload the corresponding member data of class GenericGridCollection. The discussion of base grids, refinements, component grids and multigrid coarsenings in $\S 4$ applies directly to class GridCollection. However, since each grid is a MappedGrid, we can say more about how the refinements and multigrid coarsenings are related to the base grids and component grids. In particular, each refinement must be generated by the mapping of its base grid, restricted to an aligned rectangular subset of the parameter space of the base grid. For each level-one refinement, this rectangular subset must be bounded exactly by cells of the base grid, and the cells of the refinement must refine the cells of the base grid by an integer refinement ratio in each direction, as shown in Figure 5. For each level- $n$ refinement, this rectangular subset must be bounded exactly by cells of the union of level- $(n-1)$ refinements of the same base grid, and the cells of the level- $n$ refinement must refine the cells of the level- $(n-1)$ refinements by an integer refinement ratio in each direction. While refinements of different base grids may use different refinement ratios, all same-level refinements of the same base grid must use the same refinement ratios. Each multigrid coarsenings of a component grid must be generated by the mapping of
its uncoarsened component grid (which is either a base grid or a refinement), and the cells of the level- $n$ multigrid coarsening must coarsen the cells of the level- $(n-1)$ coarsening by an integer coarsening ratio in each direction. This places a restriction on the number of cells of the component grid, namely that in each direction it must be divisible by the product of the coarsening ratios of all of its multigrid coarsenings. The member function refinementFactor returns an the refinement factor of each grid in each direction relative to its base grid; this is the product of the refinement ratios of each refinement level up to that of the grid. For example, if level-one refinement grids are refined by a ratio of two and level-two refinement grids are refined by a ratio of three, then the level-two refinement grids have a refinement factor of $6=2 \times 3$. Similarly, the member function multigridCoarseningFactor returns the multigrid coarsening factor of each grid in each direction relative to its uncoarsened component grid; this is the product of the coarsening ratios of each multigrid level up to that of the grid. Example 5 shows how some of these member functions may be used. Figure 5 shows the base grid and refinement that are produced by the example, in cases where the base grid is vertex-centered or cell-centered.

## 6 Class CompositeGrid

Class CompositeGrid is the class used for composite overlapping grids; it is a collection of MappedGrids with a description of how function values defined on the component grids are related through interpolation between component grids in their regions of overlap. Figure 6 shows a simple example of a CompositeGrid consisting of two overlapping component grids. CompositeGrid is derived from class GridCollection. It overloads some of the GridCollection public constants, member data and member functions described in $\S 5$. All of the member functions of class GridCollection described there may be used; only note that the copy constructor and the member functions reference () and operator $=()$ now take a CompositeGrid as their argument. Also, CompositeGrid overloads the member data multigridLevel, which are now a collection of CompositeGrids. Class CompositeGrid has member data that describe the criteria used in determining the overlap and interpolation of data between component grids, and the computed member data for interpolation at each interpolation point. It has member functions for use by grid-generation packages to aid in computing the overlap between component grids and determining which gridpoints should be interpolation points and from which component grid these should interpolate. Example 6 shows how some of these member data and member functions may be used.


Figure 6: An overlapping CompositeGrid. Some gridpoints are discretization points, some are interpolation points, and some gridpoints of the square grid are unused.

```
#include "CompositeGrid.h"
void example( CompositeGrid & g)
{
```

```
g.update(CompositeGrid::THEmask | // Update the interpolation data.
                CompositeGrid::THEinterpolationCoordinates | // This is usually done by a
                CompositeGrid::THEinterpoleeGrid | // grid-generation package.
                CompositeGrid::THEinterpoleeLocation |
                CompositeGrid::THEinterpolationPoint |
                CompositeGrid::THEinterpolationCondition |
                CompositeGrid::THEinverseMap);
for( Integer k=0; k<g.numberOfGrids(); k++)
{
    Integer np = g.numberOfInterpolationPoints(k); // Access the number of interpolation points,
    IntegerArray & ig = g.interpolationGrid[k], // the interpolee grids,
                                    & il = g.interpoleeLocation[k]; // the interpolee-stencil locations,
                    & ip = g.interpolationPoint[k]; // the interpolation points,
                    & ic = g.interpolationCoordinates[k];// the interpolation coordinates, and
    IntegerMappedGridFunction & mask = g. mask[k]; // the gridpoint mask.
    IntegerArray & dimension = g[k]. dimension, // Access the outer dimensions of the grid.
    Range I1(dimension(0,0), dimension(1,0)), // Construct Ranges for gridpoints in the
                I2(dimension(0,1), dimension(1,1)), // interior and on the boundary of grid k,
                I3(dimension(0,2), dimension(1,2)); // and ghost points outside the boundary.
    where (mask(I1,I2,I3) & CompositeGrid::ISdiscretizationPoint)
    {
        // ... // These are discretization points.
    }
    elsewhere (mask(I1,I2,I3) & CompositeGrid::ISinterpolationPoint)
    {
        // These are interpolation points.
    }
    elsewhere (mask(I1,I2,I3) & CompositeGrid::ISghostPoint)
    {
        // These are ghost points.
    }
    otherwise
    {
        // These are unused points.
        }
    }
}
```

Example 6: Some CompositeGrid member functions
The gridpoints of a CompositeGrid are classified as to whether they are discretization points, interpolation points, ghost points or unused points. Note that in order to make this distinction, we no longer use the terms "discretization-cell center" and "discretization point" synonymously with "gridpoint" as we did in §3.1. As before, a gridpoint is any point centered on the grid in the same way that the interior discretization stencil is centered. If the grid is vertex-centered then the gridpoints are the grid vertices, including any ghost points outside the grid boundaries; if the grid is cell-centered then the gridpoints are the grid-cell centers, including any ghost cells outside the grid boundaries. For the purposes of a CompositeGrid, "discretization-cell centers" and "discretization points" are those gridpoints in the interior or on the boundary of the grid which are labeled as discretization points in the MappedGrid member data mask, as shown in Example 6. "Interpolation points" are those interior or boundary gridpoints which are in the list of interpolation points for that grid and are labeled as interpolation points in mask. "Ghost points" are those gridpoints outside the grid boundaries for which the nearest interior or boundary gridpoint is either a discretization point or an interpolation point; ghost points are labeled as such in mask.

### 6.1 Interpolation criteria

To ensure stable and accurate interpolation of data between component grids, it is necessary to use criteria that impose some constraints on the overlap between the component grids. For example, if the interpolation points of two neighbouring component grids were perfectely aligned, then interpolation of data from each component grid to the other would consist of copying the data from the interpolation points of one component grid to those of the other and vice versa. If the interpolation points initially contained invalid data, then after interpolation they would still contain invalid data. The interpolation fails because there is insufficient overlap. With slightly more overlap, the interpolation stencils would include both interpolation points and discretization points. This is called implicit interpolation, and requires that the interpolation conditions be solved as a system of simultaneous linear equations. This system of equations becomes singular if any interpolation points of
neighbouring component grids are perfectly aligned. As the amount of overlap increases, the system of equations becomes well-conditioned. If the component grids overlap by more than half the width of the discretization stencil plus half the width of the interpolation stencil, then the interpolation stencil of each interpolation point is guaranteed to contain only discretization points of the other component grid and the system of equations becomes diagonal. This is called explicit interpolation, and allows the interpolation conditions to be applied independently at each interpolation point.

There are several CompositeGrid member data arrays and member functions that express these interpolation criteria. The array interpolationWidth indicates, for each pair of component grids at each multigrid level, the width of the interpolation stencil in each direction. The array interpolationIsImplicit indicates, for each pair of component grids at each multigrid level, whether or not the interpolation stencil for any interpolation point of the one component grid may contain interpolation points from the other component grid. If implicit interpolation is allowed, then less overlap is needed. The member functions interpolationIsAllExplicit and interpolationIsAllImplicit summarize this data, indicating whether interpolation from every pair of component grids at every multigrid level must be explicit, or whether interpolation between all pairs of component grids at all multigrid levels may be implicit. The array interpolationOverlap indicates, for each pair of component grids at each multigrid level, the minimum amount of overlap allowed in each direction. Occasionally it is useful to restrict interpolation so that interpolation is allowed only between certain pairs of grids. This constraint might be useful, for example, to avoid interpolation between grids that are known to have incompatible resolution. The array mayInterpolate indicates, for each pair of component grids at each multigrid level, whether interpolation is allowed between these component grids. In addition, it is possible to specify, for each component grid at each multigrid level, a sequence of preferences for how the gridpoints of that component grid should be used. This sequence should contain discretization as well as interpolation from any subset of the other component grids, in any sequence. For example, if discretization were specified to be the highest priority for all component grids, then the amount of overlap would be maximized, because only those points which could not be discretized would be considered for interpolation. The array interpolationPreference indicates, for each component grid at each multigrid level, the sequence of preferences for the gridpoints of that component grid. In order for gridpoints of grid $k_{1}$ to be allowed to interpolate from grid $k_{2}$, mayInterpolate $\left(k_{1}, k_{2}\right)$ must be LogicalTrue and $k_{2}$ must appear in the interpolationPreference list for $k_{1}$. These and other member data arrays and member functions that describe constraints on interpolation are summarized in Table 1.

For diagnostic purposes, class CompositeGrid allows for a second set of interpolation criteria using less stringent constraints. These are useful when no configuration of gridpoints is possible that would satisfy the primary interpolation constraints. For example, given a set of component grids with insufficient overlap, it is impossible to interpolate data between the component grids in the areas of insufficient overlap. By allowing less stringent constraints to be used where the primary constraints fail, it is possible to identify these problem areas. The parameters that describe these constraints are backupInterpolationIsImplicit, backupInterpolationWidth, backupInterpolationOverlap, backupInterpolationConditionLimit and mayBackupInterpolate. The latter determines whether the backup interpolation criteria may be used.

### 6.2 Interpolation data

The interpolation data for a CompositeGrid consists of a collection of interpolation points, with data specifying from which component grids they interpolate, and their location within the parameter space of the components grid from which they interpolate. This data may be used to compute interpolation weights. The array numberOfInterpolationPoints contains the number of interpolation points of each component grid at each multigrid level. I should discuss the following member data and functions: enum ISgivenByInterpoleePoint; IntegerArray numberOfInterpolationPoints; IntegerArray numberOfInterpoleePoints; IntegerArray interpoleeGridRange; RVector<RealArray> interpolationCoordinates; RVector<IntegerArray> interpoleeGrid; RVector<IntegerArray> interpoleePoint; RVector<IntegerArray> interpoleeLocation; RVector<IntegerArray> interpolationPoint; RVector<RealArray> interpolationCondition;

### 6.3 Local refinements and multigrid coarsenings

I should discuss the following member data and functions: IntegerArray multigridCoarseningRatio; IntegerArray multigridProlongationWidth; IntegerArray multigridRestrictionWidth; RCVector $<$ CompositeGrid $>$ multigridLevel; virtual void makeCompleteMultigridLevels(); inline void adjustBoundary(const Integer\& k1, const Integer\& k2, const IntegerArray\& i1, const RealArray\& x);

### 6.4 Miscellaneous member data and functions

I should discuss the following member data and functions: RealCompositeGridFunction inverseCondition; RealCompositeGridFunction inverseCoordinates; IntegerCompositeGridFunction inverseGrid; inline void getInterpolationStencil(const Integer\& k1, const Integer\& k2, const RealArray\& r, const IntegerArray\& interpolationStencil, const LogicalArray\& useBackupRules); inline void getInterpolationStencil(const MappedGrid\& g, const Integer\& k1, const Integer\& k2, const RealArray\& r, const IntegerArray\& interpolationStencil, const LogicalArray\& useBackupRules); inline Logical canInterpolate(const Integer\& k1, const Integer\& k2, const RealArray\& r, const LogicalArray\& ok, const LogicalArray\& useBackupRules, const Logical checkForOneSided = LogicalFalse); inline Logical canInterpolate(const MappedGrid\& g, CompositeMask\& g_mask, const Integer\& k1, const Integer\& k2, const RealArray\& r, const LogicalArray\& ok, const LogicalArray\& useBackupRules, const Logical
checkForOneSided $=$ LogicalFalse); void isInteriorBoundaryPoint(const Integer\& k1, const Integer\& k2, const IntegerArray\& i1, const RealArray\& r2, const LogicalArray\& ok); inline void adjustBoundary(const Integer\& k1, const Integer\& k2, const IntegerArray\& i1, const RealArray \& x);

## A Class ReferenceCounting

I should discuss the following member functions: the default constructor, the copy constructor, the destructor, operator $=()$, reference (), breakReference(), virtualConstructor(), incrementReferenceCount (), decrementReferenceCount(), getReferenceCount(), uncountedReferencesMayExist(), getClassName(), getGlobalID(), and consistencyCheck(). One example of a virtual member function that is overloaded in derived classes is the function getClassName(), which returns the name of the most-derived class of the object.
$\left.\begin{array}{|l|l|}\hline \hline \text { Member data or member function } & \text { Description } \\ \hline \hline \text { epsilon() } & \begin{array}{l}\text { The accuracy tolerance used in the computation of interpola- } \\ \text { tion coordinates using the inverse mapping of each component } \\ \text { grid. }\end{array} \\ \hline \text { interpolationIsImplicit }\left(k_{1}, k_{2}, l\right) \\ \text { backupInterpolationIsImplicit }\left(k_{1}, k_{2}, l\right) & \begin{array}{l}\text { LogicalTrue if interpolation of component grid } k_{1} \text { from com- } \\ \text { ponent grid } k_{2} \text { at multigrid level } l \text { may be implicit (in other } \\ \text { words, if the interpolation stencils of interpolation points of } \\ \left.\text { grid } k_{1} \text { may include interpolation points of grid } k_{2}\right) ; \text { Logical- } \\ \text { False otherwise. }\end{array} \\ \hline \text { interpolationIsAllExplicit }() & \begin{array}{l}\text { LogicalTrue if interpolationIsImplicit }\left(k_{1}, k_{2}, l\right) \text { is Logi- } \\ \text { calFalse for all pairs }\left(k_{1}, k_{2}\right) \text { of grids at all multigrid levels } l ; \\ \text { LogicalFalse otherwise. }\end{array} \\ \hline \text { interpolationIsAllImplicit }() & \begin{array}{l}\text { LogicalTrue if interpolationIsImplicit }\left(k_{1}, k_{2}, l\right) \text { is Logi- } \\ \text { calTrue for all pairs }\left(k_{1}, k_{2}\right) \text { of grids at all multigrid levels } l ; \\ \text { LogicalFalse otherwise. }\end{array} \\ \hline \begin{array}{l}\text { interpolationWidth }\left(i, k_{1}, k_{2}, l\right) \\ \text { backupInterpolationWidth }\left(i, k_{1}, k_{2}, l\right)\end{array} & \begin{array}{l}\text { The interpolation-stencil width in index direction } i \text { for interpo- } \\ \text { lation of component grid } k_{1} \text { from component grid } k_{2} \text { at multi- } \\ \text { grid level } l .\end{array} \\ \hline \begin{array}{l}\text { interpolationOverlap }\left(i, k_{1}, k_{2}, l\right) \\ \text { backupInterpolationOverlap }\left(i, k_{1}, k_{2}, l\right)\end{array} & \begin{array}{l}\text { The minimum overlap in index direction } i \text { for interpolation of } \\ \text { component grid } k_{1} \text { from component grid } k_{2} \text { at multigrid level } l .\end{array} \\ \hline \begin{array}{l}\text { interpolationConditionLimit }\left(k_{1}, k_{2}, l\right) \\ \text { backupInterpolationConditionLimit }\left(k_{1},\right.\end{array} & \begin{array}{l}\text { The maximum condition number allowed for interpolation of } \\ \text { tomponent grid } k_{1} \text { from component grid } k_{2} \text { at multigrid level } l . \\ \text { The constraint on the condition number is ignored if this pa- } \\ \text { rameter is set to zero. }\end{array} \\ \hline \text { mumberOfCompleteMultigridLevels }() & \begin{array}{l}\text { The list of preferences for interpolation and discretization of } \\ \text { component grid } k \text { at multigrid level } l . \text { For each grid } k, \text { the com- } \\ \text { ponent grid numbers of interpolee grids (and for discretization, }\end{array} \\ \text { Alhe component grid number } k) \text { are listed so that their order of } \\ \text { multigrid levels. When interpolation is updated, it is updated } \\ \text { only for the complete multigrid levels. }\end{array}\right\}$

Table 1: Some CompositeGrid member data and member functions describing the criteria used in determining interpolation and overlap between component grids

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