

OpenEye
SCIENTIFIC

Spicoli TK – Java

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Cadence Design Systems, Inc.

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CHAPTER

ONE

THEORY

The Spicoli toolkit provides broad functionality for creating, manipulating, and analyzing surfaces of many types. Surfaces can be created from molecules, grids, or other surfaces, and can be cropped, colored, and modified to enable visual and analytical analyses. The Spicoli library also provides support for saving and reading surface files.

1.1 Surfaces

In Spicoli, the surface is presented as a first-class object, i.e., an object in its own right, named *OESurface*. This presentation requires a minimalist definition similar to the way *OEChem* represents molecules as a collection of atoms and bonds. Basically, both *OESurfaces* and `OEMolBases` represent a graph in computer memory.

An *OESurface* provides two ways of retrieving data. The first is a set of methods that will return a copy of the entire underlying data array, e.g. *GetVertices*. The second is a set of methods that allow random access directly into the array of data, e.g. *GetVertex*. Basic usage of both will be shown for vertices and triangles.

1.1.1 Vertices

The simplest datum in a surface is the vertex: a set of `(x, y, z)` coordinates. Vertices are stored internally as an array of large enough to hold `GetNumVertices() * 3` floats. *Figure 1* shows how equivalent dimensions are stored at every third place in the array:

x_1	y_1	z_1	x_2	y_2	z_2	x_3	y_3	z_3	...

Fig. 1: **Figure 1**
Arrangement of coordinates in the vertices array

A copy of this array can be obtained using the code fragment in *Listing 1*, where surf is a *OESurface* object.

Listing 1: Example of retrieving the coordinates of all the vertices

```
OEFloatArray coords = new OEFloatArray(surf.GetNumVertices()*3);
surf.GetVertices(coords);
```

For direct access to the vertex array use *OESurface.GetVertex*. *Listing 2* is a code fragment that shows how to iterate over all the vertex coordinates of a surface.

Listing 2: Example of iterating over all vertices

```
OEFloatArray vert = new OEFloatArray(3);
for(int i=0; i < surf.GetNumVertices(); ++i)
{
    surf.GetVertex(i, vert);
}
```

1.1.2 Triangles

A triangle in Spicoli is a set of three vertices. However, it is important that the order of these vertices be locally consistent. To maintain this consistency vertices of the triangles are defined in a clockwise fashion.

Consider the two triangles in *Figure 2* defined by the vertices `A, B, C, D`. The triangle on the left is defined by the set `(A, B, C)`. The triangle on the right is defined by the set `(D, B, A)`. Also notice how the edge `AB` is defined in both triangles but in opposite order. This reversal of order in the two definitions is a direct consequence of the clockwise ordering rule.

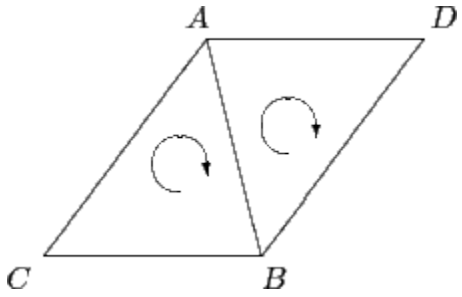


Fig. 2: **Figure 2**
Two adjacent triangles in a surface

All the methods of construction described in this document obey this rule. A surface that does not follow this rule can still be operated on by Spicoli, but it is not considered a canonical surface and some results may be incorrect or ambiguous.

Spicoli stores triangle vertices as an integer array large enough to hold `GetNumTriangles() * 3` unsigned integers. Each integer is an index into the vertex array explained in *Vertices*. *Listing 3* is a code fragment that will retrieve a copy of the entire triangles array.

Listing 3: Example of retrieving the indices of all the triangles

```
OEUIntArray triangles = new OEUIntArray(surf.GetNumTriangles()*3);
surf.GetTriangles(triangles);
```

For direct access to the triangles array use *OESurface.GetTriangle*. *Listing 4* is a code fragment that shows how to iterate over all the triangles of a surface.

Listing 4: Example of iterating over all triangles

```
OEUIntArray tri = new OEUIntArray(3);
for(int i=0; i < surf.GetNumTriangles(); ++i)
{
    surf.GetTriangle(i, tri);
}
```

1.1.3 Normal Vectors

The emphasis on triangle vertex ordering is to support the notion of the triangle's front and back. The front of the triangle is the side that the vertices appear ordered in a clockwise fashion. Surface normals can then be calculated to point out from the front of the triangle (and conversely from the back of the triangle).

The *OESurface* also supports vertex normals since vertices are often easier to work with analytically. Vertex normals are calculated by averaging all of the face normals of triangles of which the vertex is a part. The following figures contrasts the differences between face and vertex normals respectively.

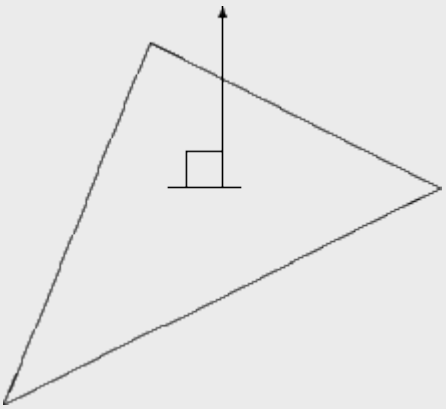


Figure 3
Face normals point out of perpendicular to the triangle

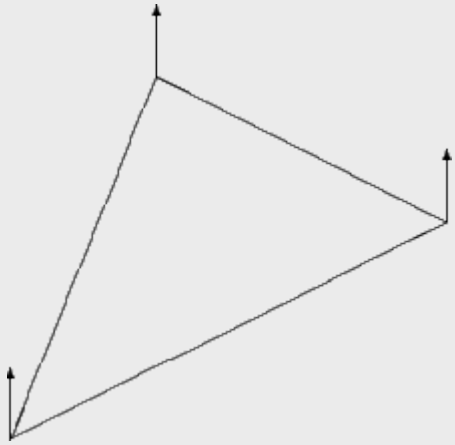


Figure 4
Vertex normals are the average of the vertices face normals

Vectors in Spicoli are represented by three floating point values. Normal vectors are always of unit length. They can be calculated and stored on a *OESurface* object by invoking the free functions `OECalculateNormals` and `OECalculateFaceNormals` for vertex and face normals, respectively.

It is important to remember that the size of a normal array is determined by whether it is a face or vertex normal. For example the size of the vertex normal array is `GetNumVertices() * 3` floats. While the size of the face normal array is `GetNumTriangles() * 3` floats.

1.1.4 Specific Data

Specific data is any information that can be derived from the surface alone but not from any one triangle or vertex. Currently these properties include the following:

Curvature
(`float`) Solvent accessibility of the vertex

Distance
(`float`) The Euclidean distance to the vertex from another portion of the surface

Curvature follows a pragmatic computational chemistry definition. It is a property of solvent molecules, represented as spheres, packed onto the surface. *Figures 5, 6, and 7* demonstrate the two dimensional case of how solvent molecules are packed onto a surface. The first sphere is mapped adjacent to the vertex using the vertex's normal. Two more spheres are then packed adjacent to the surface and the starting sphere. The angle between these two spheres is used to calculate the accessibility to solvent of the initial sphere using the following formula:

$$100 * \frac{\theta - \pi}{\pi}$$

Where θ is in radians. For this simple case the angle is also a measure of the surface curvature, hence the name. In

three dimensions steradians are required to accomplish the same functional form:

$$100 * \frac{\theta - 2\pi}{2\pi}$$

Where θ is in steradians. Therefore, a vertex's "curvature" falls into a range with the following bounds:

-100.0
Solvent that is completely secluded within the surface

0.0
Flat portion of the surface

100.0
Solvent that is completely detached from the surface

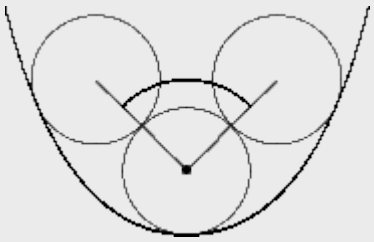


Figure 5
Concave

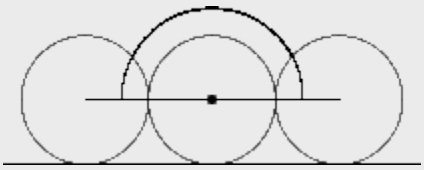


Figure 6
Flat

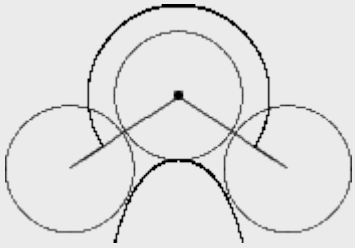


Figure 7
Convex

Distance is listed as specific data because it can be derived as the distance between different portions of the surface. This can be useful for measuring the thickness of a volume that is enclosed by a surface. Distances can also be measured to other arbitrary objects as well, such as molecules and other surfaces.

1.1.5 Associative Data

Associative data is not inherent from the first-class object definition of a surface. Instead, they are properties mapped onto the surface. Spicoli provides the following associative data arrays:

Atoms
(`unsigned int`) Atom index for the vertex

Color
(4 `floats` or 4 `unsigned chars`) Color of the vertex

Potential
(`float`) Electrostatic potential at the vertex

To map chemical properties onto a surface it is useful to know which atoms are responsible for portions of the surface. When a surface is constructed from a molecule, a data array containing the corresponding atom index for each vertex is created. An atom's index can be obtained from the `OEAtomBase.GetIdx` method and is unique over the molecule. Refer to the *OEChem* manual for more information about atom indices.

To display chemical properties it is often useful to render them as either discrete colors or a spectrum of colors. The color data array allows the user to set a color for every vertex in the surface. When the surface is then read into a visualizer, such as Vida, the properties can easily be interpreted. Every vertex has the associated values: red, green, blue, and alpha. Alpha is the transparency of the vertex. If any value is retrieved as a `float`, then that value will range from 0 to 1 inclusive. If retrieved as an `unsigned char`, the value will range from 0 to 255 inclusive.

Electrostatic potentials can be calculated and displayed on a surface. This can be done with current *OpenEye* tools such as *Zap*.

The potentials array is essentially an array of floats the user can use to record analytical data for each vertex.

1.2 Surface Generation

Spicoli can generate surfaces from the following other types of objects:

- *Molecules*
- *Grids*
- *Other Surfaces*
- *Geometric Primitives*

1.2.1 Molecules: Accessible vs Molecular

OESpicoli provides two functions for generating surfaces directly from molecules: `OEMakeAccessibleSurface` and `OEMakeMolecularSurface`. Both functions require the definition of a solvent molecule's probe radius. The default solvent is water with a probe radius of 1.4 Ångströms .

The accessible surface is created by representing each atom as a hard sphere [Lee-1971]. The radius of each sphere is the radius of the atom plus the probe radius. Figures 1 and 2 demonstrate how the spheres are packed together to form the surface. In the figures, portions of the surface are colored based upon each atom's contribution to the final accessible surface.

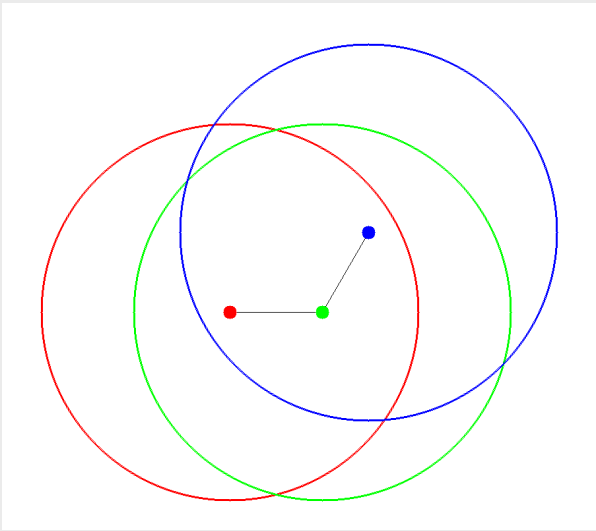


Figure 1
Accessible Spheres

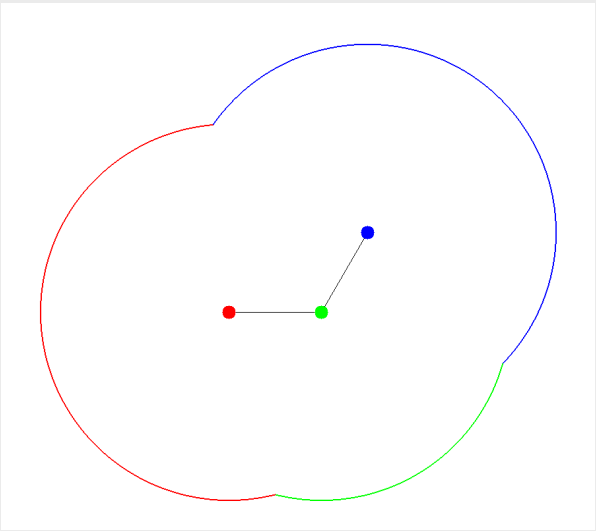


Figure 2
Accessible Surface

The molecular surface is composed of atom centered spheres plus reentrants [Connolly-1983]. Each sphere's radius is the atomic radii of the atom it is associated with. The defining characteristic of the molecular surface is the reentrant as shown in Figures 3 and 4. The reentrant models the portion of the molecule inaccessible to solvent. For this reason the volume enclosed by the molecular surface is sometimes referred to as the "solvent-excluded" volume.

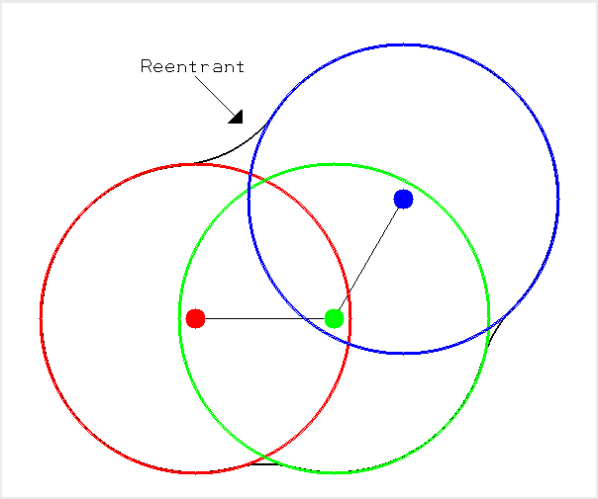


Figure 3
Molecular Spheres

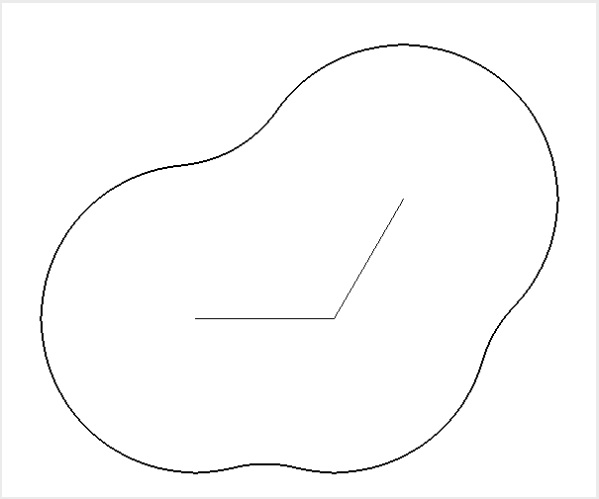


Figure 4
Molecular Surface

Note

The atoms associated with every surface vertex can be obtained by using the *OESurface.GetAtoms* and *OESurface.GetAtomsElement* methods. For an accessible surface this is simple to define, it is the atom closest to the vertex. However, for the molecular surface it is not so clear because of the re-entrants. Typically, it is the closest atom to the vertex, but that is not guaranteed. If this guarantee is required you should call the *OESurfaceToMoleculeDistance* function on the molecule and surface.

1.2.2 Grids

In Spicoli the construction of surfaces from a molecule proceeds through a grid intermediate. The space between grid points determines the resolution of the surface, i.e., how many triangles there are and the size of each triangle. Grids usually consist of equidistant points aligned along orthogonal axes, but this need not always be the case (for instance, electron density grids from crystallography).

Scalar values are placed at every grid point. Surfaces are constructed by tracing out a contour through the grid points. A contour is a separator of points based on whether they are greater than or less than a given value. The separator is a line in two dimensions and a surface in three dimensions. This is similar to how topographic maps use lines to convey elevation.

When dealing with surfaces the points on the grid with a value less than the chosen contour value are inside the surface and vice versa. *OEMakeSurfaceFromGrid* will generate a surface from a grid using a variation of the marching cubes algorithm.

Figure 5 is an example of a two dimensional molecular Gaussian grid for a simple molecule arbitrarily oriented in the grid. Figure 6 shows a contour at 1.0 of that same molecular Gaussian grid.

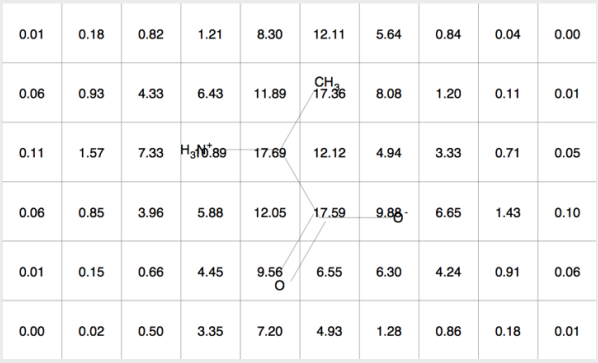


Figure 5
Molecular Gaussian Grid

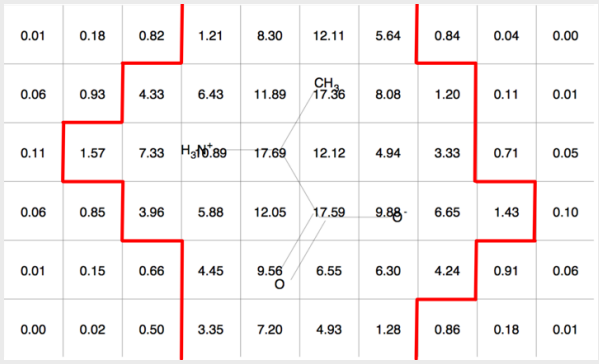


Figure 6
Molecular Gaussian Grid Contour

Note

Grids and surfaces are fairly interchangeable. A grid can be constructed from a surface using the *OEMakeGridFromSurface* function. Then that grid can be used to recreate the original surface by using the *OEMakeSurfaceFromGrid* function.

1.2.3 Surface Subsets

Surface subsetting is done through the use of *Cliques*. The triangle, not the vertex, is the most physically relevant intrinsic property of the surface. To maintain a constant surface area for the sum of all partitions Spicoli will not duplicate triangles across surface partitions. However, this does not restrict the duplication of vertices across partitions.

Therefore, the sum of the surface area of every partition will equal the surface area of the whole surface. The sum of *OESurface.GetNumTriangles* over every partition will equal the total number of triangles in the whole surface. However, the sum of *OESurface.GetNumVertices* over every partition will not equal the total number of vertices in the whole surface.

See also

- *OESurfaceCropToClique*
- *OEMakeCliqueSurface*

1.2.4 Geometric Primitives

Spicoli provides the following free functions to construct surfaces from primitive geometric shapes:

Boxes
OEMakeBoxSurface

Spheres
OEMakeSphericalSurface

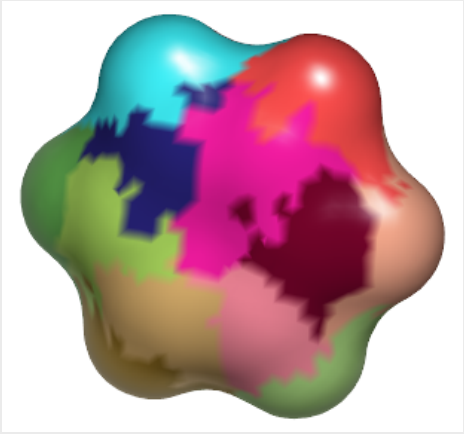
Ellipsoids
OEMakeEllipsoidSurface

1.3 Atom Association and Surface Splitting

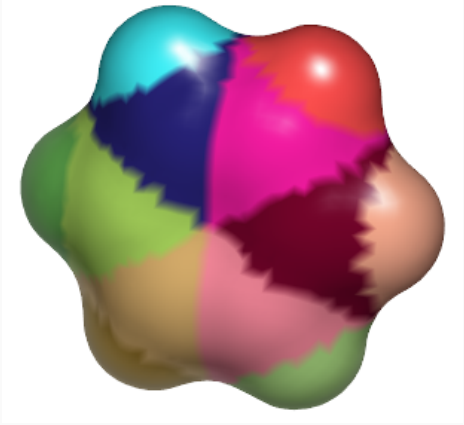
Molecular and accessible surfaces are created with an atom associated to each vertex. These atom indices can be obtained using the `OESurface.GetAtoms` and `OESurface.GetAtomsElement` methods, but the default assignments are not very accurate. Using the `OESurfaceToMoleculeDistance` function will ensure that each vertex's atom assignment is to the atom whose van der Waals surface is closest to that vertex. While the associations provide an accurate mapping of individual vertices to atoms, *triangles* on the surface may have vertices belonging to different atoms. This can make make mapping of atom-based properties onto the surface problematic.

Surface splitting, using the `OESplitSurfaceByAtoms` function, will divide a surface such that the boundaries between atoms are distinct, with no triangles being shared by multiple atoms. Surfaces are split through a process of moving vertices and subdividing triangles until no triangle edges cross the analytical boundaries between atoms. A comparison of the atom associations of unsplit and split surfaces is shown in *Table: Atom Associations*.

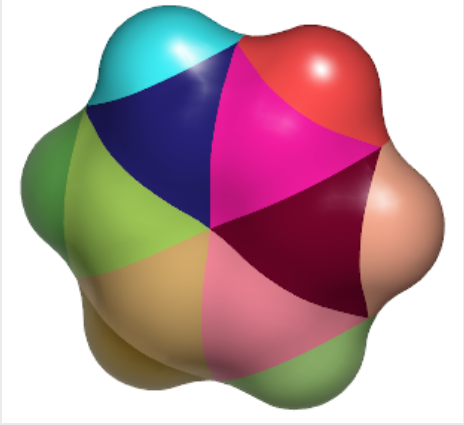
Atom Associations



Molecular surface of benzene, colored by atom indices assigned during surface construction



Same surface after atom indices are reassigned using OESurfaceToMoleculeDistance



Same surface after splitting with OESplitSurfaceByAtoms

Splitting a surface has some consequences that you should be aware of. A split surface will have significantly more vertices and triangles than the surface it was created from. In addition, it will contain numerous duplicate vertices, having the same coordinates and normals but with different atom associations. Finally, it will contain "zero-area" triangles, generated between duplicated vertices to preserve the connectivity of vertices within the surface.

1.4 Surface Manipulation

Spicoli manipulates surfaces through the following two primary mechanisms:

- *Cliques*
- *Grids*

1.4.1 Cliques

A clique is an integral value associated with portions of the surface. They can be arbitrarily assigned in order to create groupings of vertices. Cliques in Spicoli are unsigned ints that can be associated with every vertex of the surface. Spicoli treats the zero clique as a special `NULL` clique. Therefore, the user should not use zero for performing any clique operations on the surface.

Cliques in Spicoli are collections of vertices. However, an ambiguity occurs when performing triangle-based operations on these cliques. Spicoli will automatically resolve vertex cliques into triangle cliques using the following rule: if two or more vertices in the triangle have the same clique value, the triangle is assigned that clique value; otherwise, if every vertex of the triangle has a different clique value then the triangle is arbitrarily assigned the lowest clique value of the three vertices.

See also

- *OESurfaceCropToClique*
- *OEMakeCliqueSurface*
- *OEMakeConnectedSurfaceCliques*
- *OESurfaceCliqueArea*
- *OESurfaceCliqueVolume*

1.4.2 Grids

Spicoli can construct grids from surfaces. Grid values are assigned using the distance to the nearest surface vertex to the grid point. This makes grid construction very expensive because every grid point must be compared to every surface vertex. The *OEVoxelizeMethod* namespace describes the available methods.

See also

- *OEMakeGridFromSurface*
- *OEMakeSurfaceFromGrid*

1.5 Surface Storage

1.5.1 File Formats

Spicoli supports the following storage formats:

.srf
: Old GRASP format

.oesrf
: OpenEye format based upon tagged binary files

The GRASP format is provided for backwards compatibility with older visualization programs. There were byte ordering issues with the format so OpenEye developed a more flexible format based upon the tagged binary IO available in OESystem.

See also

- *OEWriteSurface*
- *OESurfaceFileType*

1.5.2 Attached to Molecules

The OpenEye format allows surfaces to be attached to molecules and then written out to OEBinary (.oeb) files. A visualizer can then read in the molecule and surface without any other means of making the association. *Listing 1* demonstrates how to properly attach surfaces to molecules.

Listing 1: Attaching a surface as generic data to be written to OEB

```
OESurface surf = new OESurface();
oespicoli.OEMakeMolecularSurface(surf, mol);
oespicoli.OESetSurface(mol, "surface", surf);

oemolostream ofs = new oemolostream("foo.oeb");
oechem.OEWriteMolecule(ofs, mol);
ofs.close();
```

Listing 2 demonstrates how to then read that surface back out of the OEB file.

Listing 2: Retrieving a surface attached as generic data from an OEB file

```
oemolistream ifs = new oemolistream("foo.oeb");
oechem.OEReadMolecule(ifs, mol);
ifs.close();

OESurface msrf = oespicoli.OEGetSurface(mol, "surface");
```

See also

- OEBase.SetData
- OEBase.GetData

Note

Versions of Spicoli prior to 1.0.2 required calling *OEInitSurfaceHandlers* in order to have surfaces attached to molecules be read and written to and from OEB.

CHAPTER

TWO

API

2.1 OESpicoli Classes

2.1.1 OESurface

```
class OESurface : public OESystem::OEBase
```

Constructors

```
OESurface()
OESurface(const OESurface& rhs)
OESurface(const OESurfaceImpl& rhs)
```

Default and copy constructors.

operator bool

```
operator bool() const
```

Whether the surface contains any data (vertices).

Clear

```
void Clear()
```

Delete and deallocate all data associated with this surface. This includes all OEBase data as well.

ClearVertexClique

```
bool ClearVertexClique()
```

Sets every vertex clique value to zero. Afterwards, *OESurface.IsVertexCliqueSet* will return `false`. This will prevent vertex clique values from being output by *OEWriteSurface*.

CreateCopy

```
OESystem::OEBase* CreateCopy() const
```

GetAtoms

```
bool GetAtoms(unsigned int* atoms) const
```

Fills the memory pointed to by `atoms` with the atom index associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices()` unsigned ints.

GetAtomsElement

```
unsigned int GetAtomsElement(unsigned int n) const
```

Retrieves an element from the internal atoms array. The index `n` should be less than `GetNumVertices()`.

GetColor

```
bool GetColor(float* color) const
bool GetColor(unsigned char* color) const
```

Fills the memory pointed to by `color` with the color associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices() * 4` floats or `GetNumVertices() * 4` unsigned chars, depending on which overload is used.

GetColorElement

```
void GetColorElement(unsigned int n, float& r, float& g, float& b,
                     float& a) const
void GetColorElement(unsigned int n, unsigned char& r,
                     unsigned char& g, unsigned char& b,
                     unsigned char& a) const
```

Retrieves an element from the internal color array. The index `n` should be less than `GetNumVertices()`.

GetCurvature

```
bool GetCurvature(float* curvature) const
```

Fills the memory pointed to by `curvature` with the curvature associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices()` floats.

GetCurvatureElement

```
float GetCurvatureElement(unsigned int n) const
```

Retrieves an element from the internal curvature array. The index `n` should be less than `GetNumVertices()`.

GetDataType

```
const void* GetDataType() const
```

GetDistance

```
bool GetDistance(float* distance) const
```

Fills the memory pointed to by `distance` with the distance each vertex is from another object. The array passed in should be large enough to hold `GetNumVertices()` floats.

GetDistanceElement

```
float GetDistanceElement(unsigned int n) const
```

Retrieves an element from the internal distance array. The index `n` should be less than `GetNumVertices()`.

GetFaceNormals

```
bool GetFaceNormals(float* faceNormals) const
```

Fills the memory pointed to by `faceNormals` with a normal vector associated with every triangle of the surface. The array passed in should be large enough to hold `GetNumTriangles() * 3` floats.

GetFaceNormal

```
bool GetFaceNormal(unsigned int n, float* normal) const
```

Retrieves a 3-component face normal vector for the specified triangle and stores it in the `normal` array. The index `n` must be less than `GetNumTriangles()`. Returns `true` upon success.

GetFaceNormalsElement

```
float GetFaceNormalsElement(unsigned int n) const
```

This method has been deprecated. Use *OESurface.GetFaceNormal* instead.

GetNormals

```
bool GetNormals(float* normals) const
```

Fills the memory pointed to by `normals` with a normal vector associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices() * 3` floats. A vertex normal is calculated by averaging the face normals of all the triangles in which the vertex resides.

GetNormal

```
bool GetNormal(unsigned int n, float* normal) const
```

Retrieves an 3-component vertex normal for the specified vertex and stores it in the `normal` array. The index `n` must be less than `GetNumVertices()`. This method returns `true` upon success.

GetNormalsElement

```
float GetNormalsElement(unsigned int n) const
```

This method has been deprecated. Use *OESurface.GetNormal* instead.

GetNumTriangles

```
unsigned int GetNumTriangles() const
```

Returns the number of triangles in the surface.

GetNumVertices

```
unsigned int GetNumVertices() const
```

Returns the number of vertices in the surface.

GetPotential

```
bool GetPotential(float* potential) const
```

Fills the memory pointed to by `potential` with the potential associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices()` floats.

GetPotentialElement

```
float GetPotentialElement(unsigned int n) const
```

Retrieves an element from the internal potentials array. The index `n` should be less than `GetNumVertices()`.

GetPotentialName

```
const char* GetPotentialName() const
```

Returns name of the potentials stored in the surface's potential array.

GetProbeRadius

```
float GetProbeRadius() const
```

Returns the probe radius used in the construction of the surface.

GetResolution

```
float GetResolution() const
```

Returns the grid spacing used in the surface construction.

GetTitle

```
const char* GetTitle() const
```

Returns the title of the surface.

GetTriangles

```
bool GetTriangles(unsigned int* triangles) const
```

Fills the memory pointed to by `triangles` with the vertex indices that compose every triangle in the surface. The vertex indices will obey the clockwise ordering rule described in the *Triangles* section. The array passed in should be large enough to hold `GetNumTriangles() * 3` unsigned ints.

GetTriangle

```
bool GetTriangle(unsigned int n, unsigned int* triangle) const
```

Retrieves the three vertex indices for the specified triangle and stores them in the `triangle` array. The triangle index `n` must be less than `GetNumTriangles()`.

GetTrianglesElement

```
unsigned int GetTrianglesElement(unsigned int n) const
```

This method has been deprecated. Use *OESurface.GetTriangle* instead.

GetVertex

```
bool GetVertex(unsigned int n, float* vertex) const
```

Retrieves coordinates for the specified vertex and stores them in the `vertex` array. The vertex index `n` must be less than `GetNumVertices()`.

GetVertexClique

```
bool GetVertexClique(unsigned int* vertexClique) const
```

Fills the memory pointed to by `vertexClique` with the clique values associated with every vertex of the surface. The array passed in should be large enough to hold `GetNumVertices()` unsigned ints.

GetVertexCliqueElement

```
unsigned int GetVertexCliqueElement(unsigned int n) const
```

Retrieves an element from the internal cliques array. The index `n` should be less than `GetNumVertices()`.

GetVertices

```
bool GetVertices(float* vertices) const
```

Fills the memory pointed to by `vertices` with the vertex coordinates of the surface. Vertices are aligned every three places in the array as described in the *Vertices* section. The array passed in should be large enough to hold `GetNumVertices() * 3` floats.

GetVerticesElement

```
float GetVerticesElement(unsigned int n) const
```

This method has been deprecated. Use *OESurface.GetVertex* instead.

IsAtomsSet

```
bool IsAtomsSet() const
```

Determine whether the surface has atom indices associated with each vertex. Surfaces generated from *OEMakeAccessibleSurface* and *OEMakeAccessibleSurface* automatically set this data.

IsColorSet

```
bool IsColorSet() const
```

Determine whether the surface has color values associated with each vertex.

IsCurvatureSet

```
bool IsCurvatureSet() const
```

Determine whether the surface has curvature value calculated for each vertex.

IsDataType

```
bool IsDataType(const void* type) const
```

IsDistanceSet

```
bool IsDistanceSet() const
```

Determine whether the surface has a distance value associated with each vertex.

IsFaceNormalsSet

```
bool IsFaceNormalsSet() const
```

Determine whether the surface has face normals calculated for each triangle.

IsNormalsSet

```
bool IsNormalsSet() const
```

Determine whether the surface has vertex normals calculated for each vertex. Surfaces generated from *OEMakeAccessibleSurface* and *OEMakeAccessibleSurface* automatically set this data.

IsPotentialSet

```
bool IsPotentialSet() const
```

Determine whether the surface has a potential value associated with each vertex.

IsVertexCliqueSet

```
bool IsVertexCliqueSet() const
```

Determine whether the surface has a clique value associated with each vertex.

SetAtoms

```
bool SetAtoms(const unsigned int* atoms)
```

Sets the internal atoms array data to the values pointed to by `atoms`. This should be a pointer to an array of unsigned ints of length `GetNumVertices()`. Returns `true` upon success.

SetAtomsElement

```
bool SetAtomsElement(unsigned int n, unsigned int value)
```

Sets an element in the internal atoms array. The index `n` should be less than `GetNumVertices()`. Returns `true` upon success.

SetColor

```
bool SetColor(const float* color)
bool SetColor(const unsigned char* color)
```

Sets the internal color array data to the values pointed to by `color`. This should be a pointer to an array of floats or unsigned chars of length `GetNumVertices() * 4` or `GetNumVertices() * 4` respectively. Returns `true` upon success.

SetColorElement

```
bool SetColorElement(unsigned int n, float r, float g, float b,
                     float a = 1.0f)
bool SetColorElement(unsigned int n, unsigned char r,
                     unsigned char g, unsigned char b,
                     unsigned char a = 255)
```

Sets an element in the internal color array. The index `n` should be less than `GetNumVertices()`. The alpha value, `a`, defaults to be opaque. Returns `true` upon success.

SetCurvature

```
bool SetCurvature(const float* curvature)
```

Sets the internal curvature array data to the values pointed to by `curvature`. This should be a pointer to an array of floats of length `GetNumVertices()`. Returns `true` upon success.

SetCurvatureElement

```
bool SetCurvatureElement(unsigned int n, float value)
```

Sets an element in the internal curvature array. The index `n` should be less than `GetNumVertices()`. Returns `true` upon success.

SetDistance

```
bool SetDistance(const float* distance)
```

Sets the internal distance array data to the values pointed to by `distance`. This should be a pointer to an array of floats of length `GetNumVertices()`. Returns `true` upon success.

SetDistanceElement

```
bool SetDistanceElement(unsigned int n, float value)
```

Sets an element in the internal distance array. The index `n` should be less than `GetNumVertices`. Returns `true` upon success.

SetFaceNormal

```
bool SetFaceNormal(unsigned int n, const float* normal)
```

Sets the face normal for the specified triangle index. The triangle index `n` must be less than `GetNumTriangles()`, and `normal` must contain three elements. Returns `true` upon success.

SetFaceNormals

```
bool SetFaceNormals(const float* faceNormals)
```

Sets the internal face normals array data to the values pointed to by `faceNormals`. This should be a pointer to an array of floats of length `GetNumTriangles() * 3`. Face normals are associated with triangles by their location in the array. Returns `true` upon success.

SetFaceNormalsElement

```
bool SetFaceNormalsElement(unsigned int n, float value)
```

This method has been deprecated. Use *OESurface.SetFaceNormal* instead.

SetNormal

```
bool SetNormal(unsigned int n, const float* normal)
```

Sets the vertex normal for the specified vertex. The vertex index `n` must be less than `GetNumVertices()`, and `normal` must contain three elements. Returns `true` upon success.

SetNormals

```
bool SetNormals(const float* normals)
```

Sets the internal vertex normals array data to the values pointed to by `normals`. This should be a pointer to an array of floats of length `GetNumVertices() * 3`. Vertex normals are associated with vertices by their location in the array. Returns `true` upon success.

SetNormalsElement

```
bool SetNormalsElement(unsigned int n, float value)
```

This method has been deprecated. Use *OESurface.SetNormal* instead.

SetNumTriangles

```
bool SetNumTriangles(unsigned int n)
```

> **Warning**
>
> Expert use only.

Set the number of triangles in this surface. Setting this to a value lower than *OESurface.GetNumTriangles* effectively erases triangles from the surface. The memory for the `OESurface` is not freed immediately, but cached for reuse.

The Clear method should be used if deallocation is desired. Deallocation is also handled automatically by the class destructor.

If the user wants to add more triangles to the surface, SetNumTriangles should be called first to resize the internal triangles array. Note that the methods for accessing individual triangles should not be used after a call to SetNumTriangles. Any data reliant on the number of triangles should first be set using the array based methods. This includes *OESurface.SetTriangles* and *OESurface.SetFaceNormals*.

SetNumVertices

```
bool SetNumVertices(unsigned int n)
```

> **Warning**
>
> Expert use only.

Set the number of vertices in this surface. Setting this to a value lower than `GetNumVertices` effectively erases vertices from the surface. The memory for the `OESurface` is not freed immediately, but cached for reuse. The *OESurface.Clear* method should be used if deallocation is desired. Deallocation is also handled automatically by the class destructor.

If the user wants to add more vertices to the surface, *OESurface.SetNumVertices* should be called first to resize the internal vertices array. Note that the methods for accessing individual vertices should not be used after a call to SetNumVertices. Any data reliant on the number of vertices should first be set using the array based methods. These include the following:

- *OESurface.SetVertices*
- *OESurface.SetNormals*
- *OESurface.SetCurvature*
- *OESurface.SetDistance*
- *OESurface.SetAtoms*
- *OESurface.SetColor*
- *OESurface.SetPotential*
- *OESurface.SetVertexClique*

SetPotential

```
bool SetPotential(const float* potential)
```

Sets the internal potential array data to the values pointed to by `potential`. This should be a pointer to an array of floats of length `GetNumVertices() * sizeof(float)`. Returns true upon success.

SetPotentialElement

```
bool SetPotentialElement(unsigned int n, float value)
```

Sets an element in the internal potential array. The index `n` should be less than `GetNumVertices()`. Returns true upon success.

SetPotentialName

```
void SetPotentialName(const char* name)
```

Set the name of the potentials that are set on the surface.

SetTitle

```
bool SetTitle(const char* title)
bool SetTitle(const std::string& title)
```

Set the title of the surface.

SetTriangle

```
bool SetTriangle(unsigned int n, const unsigned int* triangle)
```

Sets the vertex indices for the specified triangle. The triangle index `n` must be less than `GetNumTriangles()`, and `triangle` must contain three elements. Returns `true` upon success.

SetTriangles

```
bool SetTriangles(const unsigned int* triangles)
```

Sets the internal triangles array data to the values pointed to by `triangles`. This should be a pointer to an array of unsigned ints of length `GetNumTriangles() * 3`. Returns `true` upon success.

SetTrianglesElement

```
bool SetTrianglesElement(unsigned int n, unsigned int value)
```

This method is deprecated. Use *OESurface.SetTriangle* instead.

SetVertex

```
bool SetVertex(unsigned int n, const float* vertex)
```

Sets the coordinates for the specified vertex. The vertex index `n` must be less than `GetNumVertices()`, and `vertex` must contain three elements. Returns `true` upon success.

SetVertexClique

```
bool SetVertexClique(const unsigned int* vertexClique)
```

Sets the internal vertex clique array data to the values pointed to by `vertexClique`. This should be a pointer to an array of unsigned ints of length `GetNumVertices()`. Returns `true` upon success.

SetVertexCliqueElement

```
bool SetVertexCliqueElement(unsigned int n, unsigned int value)
```

Sets an element in the internal vertex clique array. The index `n` should be less than `GetNumVertices()`. Returns `true` upon success.

SetVertices

```
bool SetVertices(const float* vertices)
```

Sets the internal vertices array data to the values pointed to by `vertices`. This should be a pointer to an array of floats of length `GetNumVertices() * 3`. Returns `true` upon success.

SetVerticesElement

```
bool SetVerticesElement(unsigned int n, float value)
```

This method is deprecated. Use *OESurface.SetVertex* instead.

2.2 OESpicoli Constants

2.2.1 OEEdgeReductionType

This namespace contains constants used by the *OEReduceSurface* function.

MinimumDistance

Specifies a surface edge reduction algorithm which decreases the number of triangles and vertices in a surface by iteratively removing triangles with the shortest edges.

2.2.2 OEPolygonizeMethod

The `OEPolygonizeMethod` namespace is used to specify to the *OEMakeMolecularSurface* and *OEMakeAccessibleSurface* functions the method to be used for polygonizing the surface.

See also

- The *OEMakeMolecularSurface* and *OEMakeAccessibleSurface* functions for how to pass this constant into the functions.

Grasp

This polygonization method uses a marching cubes type of algorithm to generate surface triangles.

Compact

This polygonization method uses a variation on the marching cubes method in which grid vertex warping is used to generate a more "compact" surface. This method results in a surface which has approximately 30% fewer triangles and vertices than those generated using the *OEPolygonizeMethod.Grasp* method, with no discernible loss of quality.

Default

The default polygonization method is *OEPolygonizeMethod.Grasp*.

2.2.3 OESurfaceFileType

This namespace contains constants for passing to the *OEWriteSurface* function.

See also

- *Surface Storage*

UNDEFINED

Used to indicate errors.

Grasp

The legacy GRASP file format. Will not store all data present on the *OESurface* object.

OESurface

Binary Surface format developed by OpenEye. It will store all *OESurface* data.

2.2.4 OEVoxelizeMethod

The `OEVoxelizeMethod` namespace is used to instruct the *OEMakeGridFromSurface* function how to voxelize the surface onto the grid. A voxel is the three dimensional equivalent of a pixel.

See also

- The *OEMakeGridFromSurface* function for how to pass this constant into the function.

Distance

Each grid point is filled with the minimum distance squared from the surface. The distance is negative if the grid point is inside the surface.

Note

The distance is squared to avoid calling the costly square root function.

Gaussian

Same as distance, but the value placed in the grid is plotted as a Gaussian function. This means each gridpoint is set to $e^{-0.33*d^2}$, where d is the minimum distance to the surface. Note, where d can still be negative inside the surface. Therefore, the grid values have the following correlation to the volume enclosed by the surface:

Inside the Surface
Values are greater than 1.0

At the Surface
Values are 1.0

Outside the Surface
Values are less than 1.0 and greater than 0.0

Blank

Same as distance, but grid points inside the surface are set to 1.

Blur

Discern the shape of the volume enclosed by the surface. This is done by mapping a Gaussian for every grid point inside the volume. This smears out the surface boundary a bit and allowing a smooth drop off from the surface.

Default

The default voxelization method is *OEVoxelizeMethod.Distance*.

2.2.5 OERibbonType

The *OERibbonType* namespace is used to tell the *OEMakeProteinRibbonSurface* function what style of ribbon to create.

See also

- *OEMakeProteinRibbonSurface*

CAlpha

The ribbon is created to follow the protein backbone alpha carbons, and its helix and sheet regions will have elliptical cross-sections.

Pretty

The ribbon is created to follow the protein backbone peptide bonds, and its helix and sheet regions will have rectangular cross-sections. Ribbons created with this type tend to have a smoother, less wavy appearance.

The default ribbon type is *OERibbonType.CAlpha*.

2.3 OESpicoli Functions

2.3.1 OEAddSurfaces

```
bool OEAddSurfaces(OESurface& surf1, const OESurface& surf2)
```

Adds surf2 to surf1 using *OESurface.operator+=*. Always returns true.

2.3.2 OECalculateFaceNormals

```
bool OECalculateFaceNormals(OESurface& surf)
```

Will calculate a normal vector for every triangle of the surface and store them on the surf. To retrieve the vectors after calculation, use the *OESurface.GetFaceNormals* or *OESurface.GetFaceNormal* methods.

See also

- *Normal Vectors*

2.3.3 OECalculateNormals

```
bool OECalculateNormals(OESurface& surf)
```

Will calculate a normal vector for every vertex of the surface and store them on the surf. To retrieve the vectors after calculation, use the *OESurface.GetNormals* or *OESurface.GetNormal* methods.

See also

- *Normal Vectors*

2.3.4 OECalculateSurfaceCurvature

```
bool OECalculateSurfaceCurvature(OESurface& surf,
                                 const OEChem::OEMolBase& mol,
                                 float probeRadius = 1.4f)
```

Will calculate the surface curvature at every vertex according to the definition given in the *Specific Data* section. The data can then be retrieved using the *OESurface.GetCurvature* or *OESurface.GetCurvatureElement* methods.

The molecule passed in as `mol` is used to construct a grid marking which regions of space are inaccessible to solvent molecules. This must be the same molecule that was used to construct the surface. The molecule must have valid 3D coordinates assigned.

2.3.5 OECalculateSurfacePotentials

```
bool OECalculateSurfacePotentials(OESurface& surface,
                                  const OEChem::OEMolBase& target,
                                  const bool grasp = false)
```

Will calculate atomic potentials and assign those potentials to surface vertices on the supplied surface. The optional parameter *grasp* set to true will calculate the potentials based on the GRASP method, which is a coarser perspective of the potential using formal charges.

See also

- Atom Potentials
- *Associative Data*
- *OEColorSurfaceByPotential*

2.3.6 OECalculateTriangleAreas

```
bool OECalculateTriangleAreas(const OESurface& surf, float* areas)
```

Will calculate the area of every triangle of `surf` and store the result in the array `areas` of that should be large enough to hold `GetNumTriangles()` floats. The array is indexed by the triangle indices.

`Listing 1` demonstrates how to calculate the surface area contribution from each atom. It is assumed `surf` is an *OESurface* created from the molecule `mol`.

2.3.7 OEColorSurfaceByPotential

```
void OEColorSurfaceByPotential(OESurface& surf,
                               OESystem::OEColorGradientBase& grad,
                               const unsigned alpha = 255)
```

Method to color a surface using a defined gradient based on the stored potentials on the surface vertices.

See also

- *Associative Data*
- OEColorGradientBase

2.3.8 OEGetCenterAndExtents

```
void OEGetCenterAndExtents(const OESurface& surf, float* center,
                           float* extents)
```

Iterates through all the vertices in `surf` to find the center and extents of the surface in Cartesian coordinates. The center will be placed in the memory pointed to by `center` that should be large enough to hold 3 floats. The extents will be placed in the memory pointed to by `extents` that should be large enough to hold 3 floats. The extents are the difference between the maximum of the surface along any dimension and the minimum along that same dimension.

See also

- `OEMakeGridFromCenterAndExtents`

2.3.9 OEGetSurface

```
OESurface OEGetSurface(OEBase obj, String tag)
```

Retrieves an *OESurface* that has been stored as generic data on an OEBase object, using the specified tag.

See also

- *OESetSurface* function

2.3.10 OEGetSurfaceFileType

```
unsigned int OEGetSurfaceFileType(const char* ext)
```

Returns a constant from the *OESurfaceFileType* namespace for the file extension ext.

2.3.11 OEGetSurfaceFormatExtension

```
const char* OEGetSurfaceFormatExtension(unsigned int tag)
```

Returns a comma-separated list of possible file extensions corresponding to the specified parameter. The parameter, `tag`, should be drawn from the *OESurfaceFileType* namespace.

2.3.12 OEGetSurfaceFormatString

```
const char* OEGetSurfaceFormatString(unsigned int tag)
```

Returns the name of the file format associated with the symbolic constant `tag` from the *OESurfaceFileType* namespace.

2.3.13 OEInitSurfaceHandlers

```
void OEInitSurfaceHandlers(OEChem::oemolstreambase& fs)
bool OEInitSurfaceHandlers(OESystem::OEBinaryIOHandlerBase& b)
```

Needs to be called in order for the OEBinary writer to be able to write surfaces as generic data tagged to a molecule or any OEBase object.

Warning

Deprecated as of Spicoli 1.0.2. No longer needs to be called.

See also

- *Attached to Molecules*

2.3.14 OEInvertSurface

```
bool OEInvertSurface(OESurface& surf)
```

Reverses all the triangle orderings and normal vectors in the surface. This essentially turns the surface inside-out because all the normals facing out are turned in and vice versa.

Note

Water pockets inside of protein structures have their normals facing into the protein. This can be used to make the disconnected surface a surface enclosing the occluded water.

2.3.15 OEIsReadableSurface

```
bool OEIsReadableSurface(unsigned int type)
bool OEIsReadableSurface(const std::string& filename)
```

Returns `true` if the supplied file format is readable by Spicoli. The `filename` can be a file name or a file extension. The `unsigned int` parameter value should be drawn from the *OESurfaceFileType* namespace.

2.3.16 OEIsWriteableSurface

```
bool OEIsWriteableSurface(unsigned int type)
bool OEIsWriteableSurface(const std::string& filename)
```

Returns `true` if the supplied file format is writable by Spicoli. The `filename` can be a file name or a file extension. The `unsigned int` parameter value should be drawn from the *OESurfaceFileType* namespace.

2.3.17 OEMakeAccessibleSurface

```
bool OEMakeAccessibleSurface(OESurface& surf,
                             const OEChem::OEMolBase& mol,
                             float resolution = 0.5f,
                             float probeRadius = 1.4f,
                             unsigned int polygonizeMethod = OEPolygonizeMethod::Default)
bool OEMakeAccessibleSurface(OESurface& surf, const float* coords,
                             const float* radii, int natoms,
                             float resolution = 0.5f,
                             float probeRadius = 1.4f,
                             unsigned int polygonizeMethod = OEPolygonizeMethod::Default)
```

Fill the surface surf with the accessible surface for the molecule mol. See the *Molecules: Accessible vs Molecular* section for a full description of the accessible surface. The molecule must have valid 3D coordinates assigned. The atomic radius of each atom in the molecule should already be set before calling this function. The suggested radii can be set with `OEAssignBondiVdWRadii`.

The resolution is the grid spacing to use during surface construction. This is typically scaled with the size of the molecule. For most molecules, 0.5 is good.

The default probeRadius is 1.4 Å, the radius of water approximated as a sphere.

The `polygonizeMethod` argument specifies the method to be used when generating the triangles for the surface. Allowed values are from the *OEPolygonizeMethod* namespace.

The overloaded version of the function takes coordinate and radii arrays, `coords` and `radii` respectively, of length `natoms` to create the accessible surface.

This function will set the vertex normals and atoms arrays on the surface.

See also

- *Molecules: Accessible vs Molecular*
- The *OEPolygonizeMethod* namespace

2.3.18 OEMakeBitGridFromSurface

```
bool OEMakeBitGridFromSurface(OESystem::OEScalarGrid& grid,
                              const OESurface& surf)
bool OEMakeBitGridFromSurface(OESystem::OEScalarGrid& grid,
                              const OESurface& surf, float spacing,
                              float buffer)
```

Fill `grid` with either `0.0` or `1.0` marking whether that grid points lies inside or outside the volume enclosed by the surface. `0.0` indicates the point is outside the surface. `1.0` indicates the point is inside the surface.

2.3.19 OEMakeBoxSurface

```
bool OEMakeBoxSurface(OESurface& surf, const float* center,
                      const float* extents)
```

Creates a box in surf located at `center` and extending `extents` in each dimension. Each of the six faces of the box will be composed of two triangles.

2.3.20 OEMakeCavitySurfaces

```
bool OEMakeCavitySurfaces(const OEChem::OEMolBase& mol,
                          OESurface& surf, float resolution = 0.5f,
                          float probeRadius = 1.4f)
```

Create a surface, `surf`, from the macromolecule, `mol`, representing where solvent can be occluded inside the molecule. The molecule must have valid 3D coordinates assigned. Therefore, this will not give cavities contiguous with the outside of the molecule. The `resolution` is the grid spacing to use during surface construction. The `probeRadius` is the size of the solvent probe to use, in Angstroms.

2.3.21 OEMakeCliqueSurface

```
bool OEMakeCliqueSurface(OESurface& newsurf, const OESurface& surf,
                         unsigned int clique)
```

Creates a new surface in `newsurf` from the triangles in `surf` marked with the vertex clique value clique. Zero is not a valid clique. See the *Cliques* section on how vertex cliques are assigned to triangles. See the *Surface Subsets* section for an explanation of how Spicoli handles subset boundaries. Returns `true` if successful.

2.3.22 OEMakeComplexCavities

```
bool OEMakeComplexCavities(const OEChem::OEMolBase& mol1,
                           const OEChem::OEMolBase& mol2,
                           OESurface& surf, float resolution = 0.5f,
                           float probeRadius = 1.4f)
```

Constructs a surface representing the volume between a ligand (`mol1`) and a macromolecule (`mol2`) that can accommodate a spherical probe with radius of `probeRadius`. Both molecules must have valid 3D coordinates assigned. The resolution of the grid used to construct the surface is specified by `resolution`. The surface is restricted to a 6 Angstrom envelope around `mol1`.

2.3.23 OEMakeConnectedSurfaceCliques

```
unsigned int OEMakeConnectedSurfaceCliques(OESurface& surf)
```

Assigns a different clique value, starting at 1, to each connected component of the surface. The number of connected components is returned. *Listing 2* demonstrates cropping a surface to its largest component.

Listing 2: Extracting the largest portion of the surface

```
int nclqs = oespicoli.OEMakeConnectedSurfaceCliques(surf);

int maxclq=0;
float maxarea=0.0f;
for (int i=1; i <= nclqs; i++)
{
    float area = oespicoli.OESurfaceCliqueArea(surf, i);
    if (maxarea < area)
    {
        maxarea = area;
        maxclq = i;
    }
}
oespicoli.OESurfaceCropToClique(surf, maxclq);
```

2.3.24 OEMakeEllipsoidSurface

```
bool OEMakeEllipsoidSurface(OESurface& surf, float* center, float a,
                            float b, float c, float* dir1,
                            float* dir2, float* dir3, int level = 4)
```

2.3.25 OEMakeGridFromSurface

```
bool OEMakeGridFromSurface(OESystem::OEScalarGrid& grid,
                           const OESurface& surf,
                           unsigned int method = OEVoxelizeMethod::Default)
```

Fill `grid` with a voxelized representation of the surface by the method passed as the `method` parameter. The constants for `method` parameter are defined by the *OEVoxelizeMethod* namespace.

See also

- The *OEVoxelizeMethod* namespace.

2.3.26 OEMakeMolecularSurface

```
bool OEMakeMolecularSurface(OESurface& surf,
                            const OEChem::OEMolBase& mol,
                            float resolution = 0.5f,
                            float probeRadius = 1.4f,
                            unsigned int polygonizeMethod = OEPolygonizeMethod::Default)
bool OEMakeMolecularSurface(OESurface& surf, const float* coords,
                            const float* radii, int natoms,
                            float resolution = 0.5f,
                            float probeRadius = 1.4f,
                            unsigned int polygonizeMethod = OEPolygonizeMethod::Default)
```

Fill the surface surf with the molecular surface for the molecule mol. See *Molecules: Accessible vs Molecular* section for a full description of the molecular surface. The molecule must have valid 3D coordinates assigned. The atomic radius of each atom in the molecule should already be set before calling this function. The suggested radii can be set with `OEAssignBondiVdWRadii`.

The `resolution` is the grid spacing to use during surface construction. This is typically scaled with the size of the molecule. For most molecules 0.5 is good.

The default probeRadius is 1.4 Å, the radius of water approximated as a sphere.

The `polygonizeMethod` specifies the method to be used when generating the triangles for the surface. Allowed values are from the *OEPolygonizeMethod* namespace.

The overloaded version of the function takes a coordinate and radii array, `coords` and `radii` respectively, of length `natoms` to create the accessible surface.

This function will set the array of vertex normals and array of atom indices on the surface.

See also

- *Molecules: Accessible vs Molecular*
- The *OEPolygonizeMethod* namespace

2.3.27 OEMakeProteinRibbonSurface

```
bool OEMakeProteinRibbonSurface(OESurface& surf,
                                const OEChem::OEMolBase& mol,
                                unsigned int type = OERibbonType::CAlpha)
```

This function fills the surface surf with a ribbon surface for the molecule.

It will set the vertex normals, colors, and atom indices on the surface.

The `type` argument specifies the type of ribbon to be created, from the *OERibbonType* namespace.

2.3.28 OEMakeSphericalSurface

```
bool OEMakeSphericalSurface(OESurface& surf, float* center,
                            float radius, unsigned int level = 4)
```

Creates a spherical surface in `surf` with the center located at `center` (an array of three floats) with the radius `radius`. The `level` argument determines the number of triangles used to approximate the sphere. The number of triangles is equal to `level(level + 1) * 8`. For example the default level of 4 generates 160 triangles which is generally considered to be a good sphere to the human eye.

2.3.29 OEMakeSurfaceFromGrid

```
bool OEMakeSurfaceFromGrid(OESurface& surf,
                           const OESystem::OESkewGrid& grid,
                           float contour)
bool OEMakeSurfaceFromGrid(OESurface& surf,
                           const OESystem::OEFixedGrid<float>& grid,
                           float contour)
bool OEMakeSurfaceFromGrid(OESurface& surf,
                           const OESystem::OEFixedGrid<float>& grid,
                           float contour, float resolution)
```

An implementation of the marching cubes algorithm to create a surface, `surf`, through the values in the grid, `grid`. Grid points with values less than contour are inside the surface and the converse is true for grid points outside the surface.

See also

- The *Grids* section for more information on converting grids to surfaces.

2.3.30 OEMakeVoidVolume

```
bool OEMakeVoidVolume(const OEChem::OEMolBase& mol1,
                      const OEChem::OEMolBase& mol2,
                      OESystem::OEScalarGrid& grid, float resolution,
                      float probeRadius = 1.4f)
```

Constructs a grid representing the void, or unoccupied, volume between a ligand (`mol1`) and a macromolecule (`mol2`) that can accommodate a spherical probe with radius less than `probeRadius`. The resolution of the grid is specified by `resolution`. The grid `grid` is resized to fit a 5 Angstrom envelope around `mol1`, and its values are set to 1.0 inside the void volume and 0.0 outside.

2.3.31 OEReadSurface

```
bool OEReadSurface(const std::string& fname, OESurface& surf)
bool OEReadSurface(OEPlatform::oeistream& ifs, OESurface& surf,
                   unsigned int type)
```

Read the contents of the file named `fname` into the surface `surf`. Returns `false` if `fname` is not a valid surface file name.

An overload is provided to take any arbitrary oeistream.

2.3.32 OEReduceSurface

```
bool OEReduceSurface(OESurface& reducedSurface,
                     const OESurface& original,
                     unsigned int targetNumberOfVertices,
                     unsigned int type = OEEdgeReductionType::MinimumDistance)
```

Takes a surface and creates a new surface from it, with the new surface having a reduced number of vertices and triangles. The `targetNumberOfVertices` argument supplies a value for the desired number of vertices for the returned surface. The overall quality of the new surface will depend on this value, with smaller values giving lower quality surfaces. Currently only one edge reduction method is supported (*OEEdgeReductionType.MinimumDistance*). Returns true if the returned surface contains the requested number of vertices.

2.3.33 OERotateSurface

```
void OERotateSurface(OESurface& surf, float* rmat)
```

Rotates the surface by the supplied 3x3 matrix `rmat`, specified as a 9-element array in row-major order.

See also

- *OETranslateSurface*
- *OETransformSurface*

2.3.34 OESetSurface

```
boolean OESetSurface(OEBase obj, String tag, OESurface surface)
```

Sets an *OESurface* as generic data on an OEBase object, using the specified tag.

See also

- *OEGetSurface* function

2.3.35 OESetSurfaceColor

```
bool OESetSurfaceColor(OESurface& surf, float r, float g, float b,
                       float a = 1.0f)
bool OESetSurfaceColor(OESurface& surf, unsigned char r,
                       unsigned char g, unsigned char b,
                       unsigned char a = 255)
```

Sets the color of the entire surface to the specified color.

2.3.36 OESetSurfacePotentials

```
bool OESetSurfacePotentials(OESurface& surf,
                            const OESystem::OEScalarGrid& grid)
```

Linearly interpolates the values in the OEScalarGrid `grid` onto the surface `surf`. The scalar value associated with each vertex can then be accessed using the *OESurface.GetPotential* and *OESurface.GetPotentialElement* methods.

2.3.37 OESmoothSurfaceEdges

```
bool OESmoothSurfaceEdges(OESurface& surf)
```

Smooth the edges of an open surface by adjusting edge vertices. This is designed mostly for cleaner visual representation in 3D.

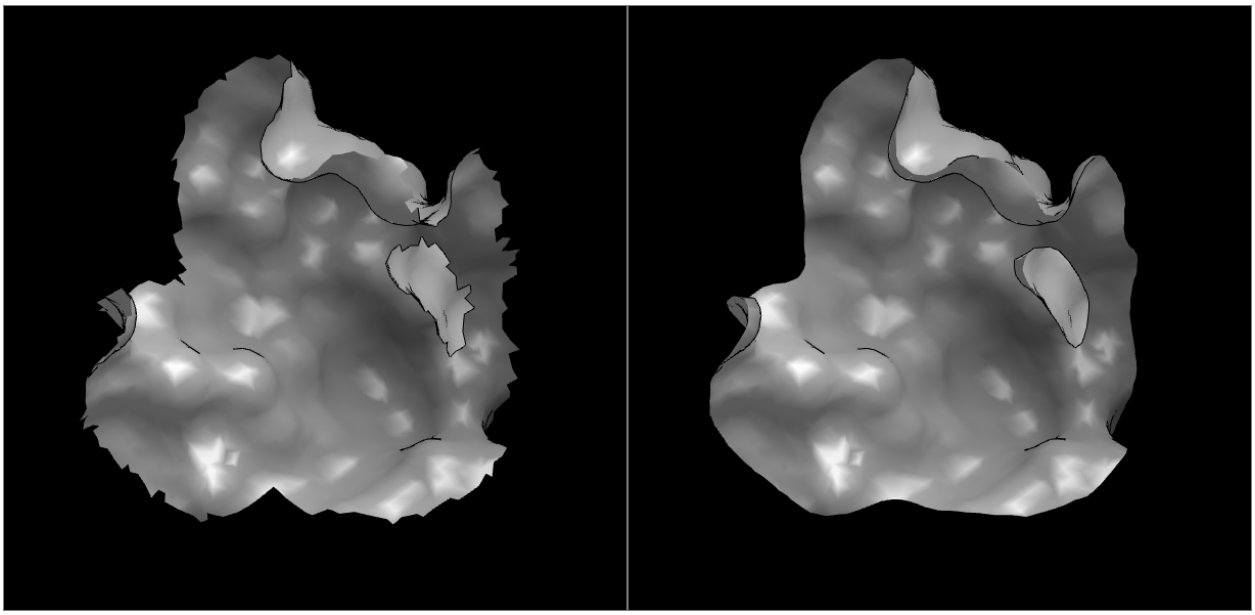


Fig. 1: Left picture is a standard, cropped subsurface. Right is the same surface after smoothing.

2.3.38 OESpicoliGetArch

```
const char* OESpicoliGetArch()
```

2.3.39 OESpicoliGetLicensee

```
bool OESpicoliGetLicensee(std::string& licensee)
```

2.3.40 OESpicoliGetPlatform

```
const char* OESpicoliGetPlatform()
```

Return the internal build string used by OpenEye Scientific Software to identify a platform. The format of these strings may change over time, and future distributions may contain different values even when using the same operating system, compiler and processor. For example, on a x86_64 Red Hat Enterprise Linux box this would return `redhat-RHEL5-g++4.1-x64`.

2.3.41 OESpicoliGetRelease

```
const char* OESpicoliGetRelease()
```

Return the release name of the OESpicoli library being used. This returns a value similar to 1.0 for production versions of the library, and 1.0 debug for the checking version of the library.

2.3.42 OESpicoliGetSite

```
bool OESpicoliGetSite(std::string& site)
```

2.3.43 OESpicoliGetVersion

```
unsigned int OESpicoliGetVersion()
```

Return the version number of the library being used. This is an unsigned integer value indicating the date on which the library was built, for example 20020903, for the 3rd of September 2002. This value should be used when reporting problems, and unlike the release string, may be used in comparisons if needed.

2.3.44 OESpicoliIsLicensed

```
bool OESpicoliIsLicensed(const char* feature = 0,
                         unsigned int* expdate = 0)
```

Determines whether a valid license file is present. This function may be called without a legitimate run-time license to determine whether it is safe to call any **Spicoli TK** functionality.

The 'feature' argument can be used to check for a valid license to **Spicoli TK** along with the following features: 'python', 'java', or 'clr' (for CSharp).

The 'expdate' argument can be used to obtain the expiration date of the current **Spicoli TK** license.

See also

- OEChemIsLicensed function

2.3.45 OESplitSurfaceByAtoms

```
bool OESplitSurfaceByAtoms(OESurface& newsurf, const OESurface& surf,
                           const OEChem::OEMolBase& mol,
                           double maxDist = 4.0)
bool OESplitSurfaceByAtoms(OESurface& surf,
                           const OEChem::OEMolBase& mol,
                           double maxDist = 4.0)
```

Given an OESurface (surf) and the molecule it was constructed from (mol), this function will create a new version of the surface with triangles cleanly partitioned by atom boundaries. The vertices, triangles, and atom associations in the surface are all adjusted from the original surface to create the partitioning. With the first form of this function, the split surface will be returned in the newsurf surface object. With the second form, the input surface is modified in-place. The maxDist parameter specifies an upper limit for the expected distance from any vertex in the surface to its assigned atom. The default value is adequate for normal molecular and solvent-accessible surfaces. Using too small of a value will result in decreased performance.

See also

- *Atom Association and Surface Splitting*

2.3.46 OESurfaceArea

```
float OESurfaceArea(const OESurface& surf)
```

Returns the total surface area of `surf`.

2.3.47 OESurfaceCliqueArea

```
float OESurfaceCliqueArea(const OESurface& surf, unsigned int clique)
```

Return the surface area for a specified clique. Zero is not a valid clique. See Section 2.3.1 on how vertex cliques are assigned to triangles.

2.3.48 OESurfaceCliqueCentroid

```
bool OESurfaceCliqueCentroid(const OESurface& surf,
                             unsigned int clique, float* centroid)
```

Return the centroid coordinates (x,y,z) in centroid for clique. Zero is not a valid clique.

See also

- The *Cliques* section on how vertex cliques are assigned to triangles.

2.3.49 OESurfaceCliqueVolume

```
float OESurfaceCliqueVolume(const OESurface& surf, unsigned int clique)
```

Return the volume for a specified clique. Zero is not a valid clique.

See also

- The *Cliques* section on how vertex cliques are assigned to triangles.

Note

The volume may be negative if the clique is an open surface. However, the sum of all surface partitions will equal the total volume of the enclosed surface.

2.3.50 OESurfaceCropToClique

```
bool OESurfaceCropToClique(OESurface& surf, unsigned int clique)
```

Trim surf of the triangles not marked with the vertex clique value clique. Zero is not a valid clique. See Section 2.3.1 on how vertex cliques are assigned to triangles. Returns true if successful.

See also

- The *Cliques* section on how vertex cliques are assigned to triangles.
- The *Surface Subsets* section for an explanation of how Spicoli handles subset boundaries.

2.3.51 OESurfaceIsOpen

```
bool OESurfaceIsOpen(const OESurface& surf)
```

Returns whether the surface is open. A surface is open if any triangle does not border exactly three other triangles.

2.3.52 OESurfaceToMoleculeDistance

```
bool OESurfaceToMoleculeDistance(OESurface& surf,
                                 const OEChem::OEMolBase& mol)
```

Will calculate the minimum distance between every vertex in the surface (surf) and every atom in the molecule (mol). The molecule must have valid 3D coordinates assigned. The minimum distance for each vertex is then stored on the surface to be accessed via the *OESurface.GetDistance* and *OESurface.GetDistanceElement* methods. Distances are calculated as the euclidean distance between the vertex and atom center minus the atomic radii. Note that this can result in distances that are negative to denote that they are `inside` the molecule. If atomic radii are not specified on the molecule BondiVdWRadii will be used.

This function will also reassign the atom indices associated with every vertex of the surface. To access these changes use the *OESurface.GetAtoms* and *OESurface.GetAtomsElement* methods.

2.3.53 OESurfaceVolume

```
float OESurfaceVolume(const OESurface& surf)
```

Returns the volume enclosed by the surface.

2.3.54 OETransformSurface

```
void OETransformSurface(OESurface& surf, const OEChem::OETrans& trans)
```

Transforms a surface using a supplied OETrans object.

See also

- *OERotateSurface*
- *OETranslateSurface*
- OETrans

2.3.55 OETranslateSurface

```
void OETranslateSurface(OESurface& surf, float* trans)
```

Translates the surface using the supplied 3-element translation vector.

See also

- *OERotateSurface*
- *OETransformSurface*

2.3.56 OEWriteSurface

```
bool OEWriteSurface(const std::string& fname, const OESurface& surf)
bool OEWriteSurface(OEPlatform::oeostream& ofs, const OESurface& surf,
                    unsigned int type)
```

Write surf to the surface file `fname`. Returns `false` if `fname` is not a valid surface file name. This will overwrite the previous file if it existed.

The overload that takes an `oeostream` can be used to write multiple surfaces to the same destination. Note that the format must be specified by a constant from the *OESurfaceFileType* namespace as the type argument. The *OESurfaceFileType.Grasp* format does not support this kind of use. Returns `true` if written successfully.

CHAPTER

THREE

RELEASE HISTORY

3.1 Spicoli TK 1.6.4

Minor internal improvements have been made.

3.2 Spicoli TK 1.6.3

Minor internal improvements have been made.

3.3 Spicoli TK 1.6.2

Minor internal improvements have been made.

3.4 Spicoli TK 1.6.1

Minor internal improvements have been made.

3.5 Spicoli TK 1.6.0

Minor internal improvements have been made.

3.6 Spicoli TK 1.5.7

3.6.1 New features

- A function was added to assign surface potentials based on a molecule's *OECalculateSurfacePotentials*, using either atomic potentials or a potential based on formal charges of protein residues at the protein surface (GRASP) using Zap (license required).
- A function was added to color a surface based on its stored potential *OEColorSurfaceByPotential*.

3.7 Spicoli TK 1.5.6

Minor internal improvements have been made.

3.8 Spicoli TK 1.5.5

Minor internal improvements have been made.

3.9 Spicoli TK 1.5.4

- Minor internal improvements have been made.

3.10 Spicoli TK 1.5.3

Fall 2021

- Minor internal improvements have been made.

3.11 Spicoli TK 1.5.2

July 2021

Minor internal improvements have been made.

3.12 Spicoli TK 1.5.1

Fall 2020

- Minor internal improvements have been made.

3.13 Spicoli TK 1.5.0

- Minor internal improvements have been made.

3.14 Spicoli TK 1.4.7

- Minor internal improvements have been made.

3.15 Spicoli TK 1.4.6

- Minor internal improvements have been made.

3.16 Spicoli TK 1.4.5

3.16.1 New features

- DNA/RNA ribbons are now available through the `OEMakeProteinRibbonSurface` function. When molecules containing DNA or RNA residues are passed to this function with a ribbon style of `OERibbonType.Pretty`, the resulting surface now contains ribbons for both protein and nucleic acid residues.

3.16.2 Major bug fixes

- *OEMakeAccessibleSurface* no longer crashes when passed extremely large molecules (many hundreds of Angstroms across). The function now reduces the resolution of the surface, if necessary, to allow the surface to fit in the available memory.

3.17 Spicoli TK 1.4.4

- Minor internal improvements have been made.

3.18 Spicoli TK 1.4.3

3.18.1 Minor bug fixes

- A bug that caused protein ribbons created with the type *OERibbonType.Pretty* to be truncated by one residue at the C-terminus has been fixed.

3.19 Spicoli TK 1.4.2

3.19.1 New features

- A new style of protein ribbons has been added and is accessible through the function *OEMakeProteinRibbonSurface*. A third argument, a constant from the *OERibbonType* namespace, has been added to this function to specify the ribbon type. The new ribbon style *OERibbonType.Pretty* creates ribbons that have a smoother appearance than the older, default style.

3.19.2 Major bug fixes

- A crash that occurred with calling one variant of *OEMakeBitGridFromSurface* has been fixed.

3.20 Spicoli TK 1.4.1

- Minor internal improvements have been made.

3.21 Spicoli TK 1.4.0

3.21.1 Minor bug fixes

- A crash in the *OEMakeProteinRibbonSurface* function that occurred when adding a ribbon to proteins with C-alpha atoms and alternate locations has been fixed.

3.22 Spicoli TK 1.3.7

- Minor internal improvements have been made.

3.23 Spicoli TK 1.3.6

3.23.1 New features

- *OESmoothSurfaceEdges* function has been added for cleaner visual representation in 3D.

3.23.2 Major bug fixes

- A crash in *OEMakeGridFromSurface* has been fixed. The crash occurred when the function was passed a grid that wasn't large enough to enclose the entire surface.

3.24 Spicoli TK 1.3.5

3.24.1 Major bug fixes

- Surface readers have been made more robust to junk data being passed to them. They should no longer crash for any random data input.

3.24.2 Documentation changes

- The `anisotropy` example has been updated to perceive residues in cases when it is not done by the molecule reader (for example, in the case of `mol2`).

3.25 Spicoli TK 1.3.4

- Minor internal cleanup has been performed.

3.26 Spicoli TK 1.3.3

3.26.1 Minor bug fixes

- Internal refactoring has been performed to improve stability.

3.26.2 Documentation fixes

- *OESetSurface* and *OEGetSurface* documentation have been added for Python, Java, and C#.
- The *OEEdgeReductionType* namespace is now documented.
- The missing Java example Volume.java has been added.

3.27 Spicoli TK 1.3.2

- *OEMakeCliqueSurface* and *OESurfaceCropToClique* will no longer leave the *OESurface* consuming more memory than necessary.
- The following examples have been added to the Java distribution:
  - PsaSurface.java
  - Cavities.java
  - ComplexCavities.java
  - BindingSite2.java
  - BindingSite1.java

3.28 Spicoli TK 1.3.1

3.28.1 New features

- *OEMakeComplexCavities* added a "probe radius" argument. Previously, the probe radius used in the calculation was always set to 1.4 Angstroms.
- *OEMakeProteinRibbonSurface* added to generate a protein ribbon as an *OESurface* object.

3.28.2 Documentation fixes

- *OEMakeVoidVolume* documentation corrected to clarify the meaning of the probe radius argument.
- Java examples have been added to demonstrate additional functionality.

3.29 Spicoli TK 1.3.0

3.29.1 New features

- The internals of the Spicoli toolkit have been migrated from C to pure C++ to ensure better interoperability with C++, especially in terms of object lifetime and management.

For Java, this means explicitly calling the *OESurface::delete()* method should no longer be required to avoid a race condition with the Java finalizer thread. This should make working with *OESurface* objects feel much more natural in Java.

- A new function, OESplitSurfaceByAtoms, will divide an OESurface and cleanly partition the triangles along atom boundaries. The result is a surface that can be nicely divided and colored by its underlying atoms.
- The OESurface class has a new method, GetProbeRadius, which returns the probe radius value used to create the surface.
- The functions OEMakeCavitySurfaces and OEMakeVoidVolume now accept an optional probe radius parameter to be used for the surface construction. The default value of this parameter is 1.4 Angstroms.

3.29.2 Minor bug fixes

- Generic data stored on an OESurface is now saved when the surface is written to .oeb or .oesrf files.

3.30 Spicoli TK 1.2.2

- Minor internal improvements.

3.31 Spicoli TK 1.2.1

- Minor internal improvements.

3.32 Spicoli TK 1.2.0

- A number of *OESurface* methods for accessing triangles, vertices, and normals have been deprecated and replaced with more convenient methods. The old methods required three calls to get all three components of a vector or triangle, while the new methods only require one.

Deprecated Methods	Replacement Methods
GetVerticesElement	GetVertex
SetVerticesElement	SetVertex
GetTrianglesElement	GetTriangle
SetTrianglesElement	SetTriangle
GetNormalsElement	GetNormal
SetNormalsElement	SetNormal
GetFaceNormalsElement	GetFaceNormal
SetFaceNormalsElement	SetFaceNormal

- A new polygonization method has been made available to the *OEMakeMolecularSurface* and *OEMakeAccessibleSurface* functions. An optional argument to these functions can specify *OEPolygonizeMethod.Grasp* (the original method) or *OEPolygonizeMethod.Compact* (the newer method). The newer method produces surfaces with around 30% fewer triangles and vertices, and a more uniform spacing of vertices. The argument defaults to the original method, so existing code won't be affected.
- *OEReduceSurface* added that allows the reduction of the number of vertices in a surface to a user-specified number.
- New functions have been provided for transforming *OESurface* coordinates and normals: *OERotateSurface*, *OETranslateSurface*, and *OETransformSurface*.

3.33 Spicoli TK 1.1.3

- Internal build system improvements.

3.34 Spicoli TK 1.1.2

- Internal build system improvements.

3.35 Spicoli TK 1.1.1

3.35.1 Bug fixes

- Minor documentation fixes.
- *OEMakeComplexCavities* example program now properly suppresses hydrogen and passes the protein and ligand to the function in the proper order.
- *OEMakeVoidVolume* is now usable in Java, the signature used to use an incorrect grid type.
- Surface IO APIs now properly wrapped in Java.

3.36 Spicoli TK 1.1.0

3.36.1 New Features

- Added the *OEMakeBitGridFromSurface* function. This is a lot faster than using *OEMakeGridFromSurface* to generate a lookup grid for whether a point is inside or outside a surface.
- Added *OESetSurface* and *OEGetSurface* to the Java wrappers.

See also

- *Attached to Molecules*

3.36.2 Bug fixes

- The previous release (1.0.2) introduced the feature that didn't require the user to call *OEInitSurfaceHandlers*. This didn't work sometimes when statically linking an executable. This was because the library initialization code that needed to get run was getting discarded by the linker because none of the functions in that translation unit were being called. The library initialization code has been migrated to the same translation unit as the *OESurface* since these functions always have to be called to attach a molecule as generic data.

Note

This only affected C++ users.

3.37 Spicoli TK 1.0.2

3.37.1 New features

- The user is no longer required to call *OEInitSurfaceHandlers* in order to attach surfaces to molecules and then write them out to OEB. This occurs at library link time now.

3.37.2 Minor bug fixes

- *OESurface.operator=* now copies the OEBase data.
- *OEMakeCliqueSurface* and *OESurfaceCropToClique* now preserve OEBase data.

3.38 Spicoli TK 1.0.1

3.38.1 Bug fixes

- *OEInvertSurface* properly inverts all surface normals.
- *OEMakeCavitySurfaces* was totally busted before. Added a default resolution of 0.5.
- Added a default resolution of 0.5 to *OEMakeComplexCavities*.
- *OEMakeBoxSurface* now takes a `const float *` as it should.

CHAPTER

FOUR

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CHAPTER

FIVE

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CHAPTER

SIX

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```

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```
Orion 2025.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com.
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The version number for Orion appears in the product's release notes, for example, https://docs.eyesopen.com/orion-user-interface/releasenotes/index.html.

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OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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The Applications and Toolkits are released as a package, multiple times per year. The first part of the version number designates the calendar year. The version number appears on the summary document for the package.

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- Bioisostere TK
- OEChem TK
- OEDepict TK
- OEDocking TK
- OEFF TK
- Eon TK
- FastROCS TK
- Grapheme TK
- GraphSim TK
- Lexichem TK
- OEMedChem TK
- MolProp TK
- Omega TK
- Quacpac TK
- Shape TK
- Spicoli TK
- Spruce TK
- Szmap TK
- Szybki TK
- Zap TK
- AFITT Application
- BROOD Application
- OEDocking Application
- EON Application
- OMEGA Application
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- SPRUCE Application
- SZMAP Application
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You can use the version number of the individual Application or Toolkit. For example:

```
SZYBKI Application 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://
↪www.eyesopen.com.

Szybki TK 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The first documentation pages give the product names and version numbers, as in https://docs.eyesopen.com/applications/szybki/index.html and https://docs.eyesopen.com/toolkits/python/szybkitk/index.html.

6.4 Publications for Bibliographies

Please also cite these publications if the corresponding product was used in your research.

6.4.1 Orion

Sørensen, J., Bannan, C.C., Calabrò, G., Jain, V., Ovanesyan, G., Smith, A., Zhang, S., Bayly, C.I., Darden, T.A., Geballe, M.T., LeBard, D.N., McGann, M., Moon, J.B., Muddana, H.S., Shewmaker, A., LaFon, J., Tolbert, R.W., Skillman, A.G., Nicholls, A. Orion® A Cloud-Native Molecular Design Platform. In *Computational Drug Discovery*. V. Poongavanam and V. Ramaswamy, Eds. Wiley-VCH, 2024; pp. 579–615. DOI: 10.1002/9783527840748.ch24

6.4.2 AFITT and FLYNN Applications

Wlodek, S.; Skillman, A.G.; Nicholls, A. Automated Ligand Placement and Refinement with a Combined Force Field and Shape Potential. *Acta Crystallogr., Sect. D: Struct. Biol.* **2006**, *62* (7), 741–749. DOI: 10.1107/s0907444906016076

6.4.3 OEDocking Application and Toolkit

Kelley, B.P.; Brown, S.P.; Warren, G.L.; Muchmore, S.W. POSIT: Flexible Shape-Guided Docking For Pose Prediction. *J. Chem. Inf. Model.* **2015**, *55* (8), 1771-1780. DOI: 10.1021/acs.jcim.5b00142

McGann, M. FRED Pose Prediction and Virtual Screening Accuracy. *J. Chem. Inf. Model.* **2011**, *51* (3), 578-596. DOI: 10.1021/ci100436p

McGann, M. FRED and HYBRID Docking Performance on Standardized Datasets. *J. Comput.-Aided Mol. Des.* **2012**, *26* (8), 897-906. DOI: 10.1007/s10822-012-9584-8

6.4.4 OMEGA Application and Toolkit

If you are using OMEGA in torsion driving mode, please cite the following two publications.

Hawkins, P.C.D.; Skillman, A.G.; Warren, G.L.; Ellingson, B.A.; Stahl, M.T. Conformer Generation with OMEGA: Algorithm and Validation Using High Quality Structures from the Protein Databank and the Cambridge Structural Database. *J. Chem. Inf. Model.* **2010**, *50* (4), 572-584. DOI: 10.1021/ci100031x

Hawkins, P.C.D. and Nicholls, A. Conformer Generation with OMEGA: Learning from the Data Set and the Analysis of Failures. *J. Chem. Inf. Model.* **2012**, *52* (11), 2919–2936. DOI: /10.1021/ci300314k

If you are using OMEGA in macrocyle mode, please cite the following.

Hawkins, P.C.D. and Wlodek, S. Decisions with Confidence: Application to the Conformation Sampling of Molecules in the Solid State. *J. Chem. Inf. Model.* **2020**, *60* (7), 3518–3533. DOI: /10.1021/acs.jcim.0c00358

6.4.5 ROCS Application

Hawkins, P.C.D.; Skillman, A.G.; Nicholls, A. Comparison of Shape-Matching and Docking as Virtual Screening Tools. *J. Med. Chem.* **2007**, *50* (1), 74-82. DOI: 10.1021/jm0603365

6.5 OpenEye MMDS Web Service

To cite use of the Macromolecular Data Service (MMDS) web service, please use the syntax:

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Macromolecular Data Service <version-number>. OpenEye, Cadence Molecular Sciences, Santa␣
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The MMDS version number appears on the web service's release notes.

CHAPTER

SEVEN

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arrow	https://github.com/arrow-py/arrow	https://github.com/arrow-py/arrow?tab=Apache-2.0-1-ov-file#readme
ascii85	https://github.com/huandu/node-ascii85	https://github.com/huandu/node-ascii85/raw/master/LICENSE
ase	https://wiki.fysik.dtu.dk/ase/	https://wiki.fysik.dtu.dk/ase/development/licenseinfo.html#license-info
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blosc2	https://github.com/Blosc/python-blosc2	https://github.com/Blosc/c-blosc2/blob/main/LICENSE.txt

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boltons	https://github.com/mahmoud/boltons	https://github.com/mahmoud/boltons/blob/master/LICENSE
Boltz	https://boltz.bio	https://github.com/jwohlwend/boltz/blob/main/LICENSE
boost	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
boost-cpp	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue/raw/master/LICENSE
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brotlipy	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE

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bson	http://github.com/py-bson/bson	https://github.com/py-bson/bson/blob/master/LICENSE_APACHE
bytefmt	https://code.cloudfoundry.org/bytefmt	https://github.com/cloudfoundry/bytefmt/blob/master/LICENSE
bzip2	https://www.bzip.org	https://spdx.org/licenses/bzip2-1.0.6.html
c-ares	https://github.com/c-ares/c-ares	https://github.com/c-ares/c-ares/blob/main/LICENSE.md
ca-certificates	https://github.com/conda-forge/ca-certificates-feedsto	https://wiki.mozilla.org/CA/Included_Certificates
cached-property	https://github.com/pydanny/cached-property	https://github.com/pydanny/cached-property/blob/master/LICENSE
cachetools	https://github.com/tkem/cachetools/	https://github.com/tkem/cachetools/blob/master/LICENSE
cairo	https://pycairo.readthedocs.io/en/latest/	https://github.com/pygobject/pycairo/blob/master/COPYING
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cctbx	https://github.com/cctbx/cctbx_project	https://github.com/cctbx/cctbx_project/blob/master/cctbx/LICENSE_2_0.txt
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Cerberus	https://docs.python-cerberus.org/en/stable/	https://docs.python-cerberus.org/en/stable/license.html
certifi	https://certifiio.readthedocs.io/en/latest/	https://wiki.mozilla.org/index.php?title=CA/IncludedCertificates&redirect=no

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ChEMBL Structure Pipeline	https://github.com/chembl/ChEMBL_Structure_Pipeline/tree/master	https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/LICENSE
choreographer	https://github.com/mazpie/choreographer	https://github.com/mazpie/choreographer/blob/main/LICENSE
chunkreader	https://github.com/jackc/chunkreader/v2	https://github.com/jackc/chunkreader/blob/master/LICENSE
click	https://palletsprojects.com/p/click/	https://github.com/pallets/click/blob/main/LICENSE.rst
click-completion	https://github.com/click-contrib/click-completion	https://github.com/click-contrib/click-completion/blob/master/LICENSE
click-didyoumean	https://github.com/click-contrib/click-didyoumean	https://github.com/click-contrib/click-didyoumean/blob/master/LICENSE
click-plugins	https://github.com/click-contrib/click-plugins	https://github.com/click-contrib/click-plugins/blob/master/LICENSE.txt

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Name of Project	Website	License URL
click-repl	https://github.com/untitaker/click-repl	https://github.com/click-contrib/click-repl/blob/master/LICENSE
cloudpickle	https://github.com/cloudpipe/cloudpickle	https://github.com/cloudpipe/cloudpickle/blob/master/LICENSE
cmake	https://cmake.org/	https://cmake.org/licensing/
colorama	https://github.com/tartley/colorama	https://github.com/tartley/colorama/blob/master/LICENSE.txt
comm	https://github.com/ipython/comm	https://github.com/ipython/comm/blob/master/LICENSE
compose	https://github.com/docker/compose	https://github.com/docker/compose/blob/v2/LICENSE
conda-content-trust	https://github.com/conda/conda-content-trust	https://github.com/conda/conda-content-trust/blob/main/LICENSE
conda-libmamba-solver	https://github.com/conda/conda-libmamba-solv	https://github.com/conda/conda-libmamba-solv/blob/main/LICENSE
conda-pack	https://conda.github.io/conda-pack/	https://github.com/conda/conda-pack/blob/main/LICENSE.txt
conda-package-handling	https://github.com/conda/conda-package-handli	https://github.com/conda/conda-package-handli/blob/main/LICENSE
conda-package-streaming	https://anaconda.org/conda-forge/conda-package-stream	https://github.com/conda/conda-package-stream/blob/main/LICENSE
conda-token	https://anaconda.org/anaconda/conda-token	https://anaconda.org/anaconda/conda-token

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Name of Project	Website	License URL
conda_package_strear	https://github.com/conda/conda-package-streamtree/main/conda_package_streaming	https://github.com/conda/conda-package-streamtab=License-1-ov-file
confuse	https://github.com/beetbox/confuse	https://github.com/beetbox/confuse/blob/main/LICENSE
contourpy	https://github.com/contourpy/contourpy	https://github.com/contourpy/contourpy/blob/main/LICENSE
cpp-expected	https://github.com/TartanLlama/expected	https://github.com/TartanLlama/expected?tab=CC0-1.0-1-ov-file#readme
cpp-peglib	https://github.com/yhirose/cpp-peglib	https://github.com/yhirose/cpp-peglib/blob/master/LICENSE
cryptography	https://github.com/pyca/cryptography	https://github.com/pyca/cryptography/blob/main/LICENSE
cssselect2	https://github.com/Kozea/cssselect2/	https://github.com/Kozea/cssselect2/blob/master/LICENSE
cuda-bindings	https://nvidia.github.io/cuda-python/cuda-bindings/latest/install.html	https://github.com/NVIDIA/cuda-python/blob/main/cuda_bindings/LICENSE
cuda-pathfinder	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/	https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/license.html
cudatoolkit	https://developer.nvidia.com/cuda-toolkit	https://docs.nvidia.com/cuda/eula/index.html
cuequivariance-ops-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE

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Name of Project	Website	License URL
cuequivariance-ops-torch-cu12	https://developer.nvidia.com/cuequivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cuequivariance-torch	https://docs.nvidia.com/cuda/cuequivariance/	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
cupy-cuda113	https://cupy.dev/	https://github.com/cupy/cupy/blob/main/LICENSE
cupy-cuda11x	https://cupy.dev/	https://github.com/cupy/cupy/?tab=MIT-1-ov-file#readme
curl	https://curl.se	https://curl.se/docs/copyright.html
cycler	https://github.com/matplotlib/cycler	https://github.com/matplotlib/cycler/blob/main/LICENSE
cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl	https://github.com/cyrusimap/cyrus-sasl/blob/master/COPYING
Cython	https://cython.org	https://www.apache.org/licenses/LICENSE-2.0.html
d3	https://github.com/mbostock/d3	https://github.com/mbostock/d3/raw/master/LICENSE
dataclasses	https://github.com/ericvsmith/dataclasses	https://github.com/ericvsmith/dataclasses/blob/master/LICENSE.txt
ddsketch	http://github.com/datadog/sketches-py	https://github.com/DataDog/sketches-py/blob/master/LICENSE
debugpy	https://aka.ms/debugpy	https://github.com/microsoft/debugpy/blob/main/LICENSE

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Name of Project	Website	License URL
decimal	https://github.com/shopspring/decimal	https://github.com/shopspring/decimal/blob/master/LICENSE
decorator	https://github.com/micheles/decorator	https://github.com/micheles/decorator/blob/master/LICENSE.txt
deepdiff	https://github.com/seperman/deepdiff	https://github.com/seperman/deepdiff/blob/master/LICENSE
deeptime	https://github.com/deeptime-ml/deeptime	https://github.com/deeptime-ml/deeptime/blob/main/LICENSE.txt
defusedxml	https://github.com/tiran/defusedxml	https://github.com/tiran/defusedxml/blob/main/LICENSE
dftd3	https://github.com/dftd3/tad-dftd3	https://github.com/dftd3/tad-dftd3/blob/main/LICENSE
dill	https://github.com/uqfoundation/dill	https://github.com/uqfoundation/dill/blob/master/LICENSE
distlib	https://distlib.readthedocs.io/en/latest/	https://github.com/pypa/distlib/blob/master/LICENSE.txt
distro	https://github.com/python-distro/distro	https://github.com/python-distro/distro/blob/master/LICENSE
Django	https://www.djangoproject.com/	https://github.com/django/django/blob/main/LICENSE
django-classy-tags	https://github.com/django-cms/django-classy-tags	https://github.com/django-cms/django-classy-tags/blob/master/LICENSE
django-cors-headers	https://github.com/adamchainz/django-cors-headers	https://github.com/adamchainz/django-cors-headers/blob/main/LICENSE

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Name of Project	Website	License URL
django-csp	https://github.com/mozilla/django-csp	https://github.com/mozilla/django-csp/blob/main/LICENSE
django-extensions	https://github.com/django-extensions/django-extensions	https://github.com/django-extensions/django-extensions/blob/main/LICENSE
django-filter	https://github.com/carltongibson/django-filter/tree/master	https://github.com/carltongibson/django-filter/blob/main/LICENSE
django-redis	https://github.com/jazzband/django-redis	https://github.com/jazzband/django-redis/blob/master/LICENSE
django-taggit	https://github.com/jazzband/django-taggit	https://github.com/jazzband/django-taggit/blob/master/LICENSE
django-taggit-serializer	https://github.com/glemmaPaul/django-taggit-serializ	https://github.com/glemmaPaul/django-taggit-serializ blob/master/LICENSE
django-taggit-templatetags2	https://github.com/fizista/django-taggit-templat	https://github.com/fizista/django-taggit-templat blob/master/LICENSE.txt
djangorestframework	https://www.django-rest-framewor org/	https://github.com/encode/django-rest-framewor blob/master/LICENSE.md
dkh	https://psicode.org/psi4manual/master/dkh.html	https://github.com/psi4/dkh/blob/master/COPYING.LESSER
dm-tree	https://github.com/deepmind/tree	https://github.com/deepmind/tree/blob/master/LICENSE
docker-py	https://github.com/docker/docker-py/	https://github.com/docker/docker-py/blob/master/LICENSE

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Name of Project	Website	License URL
docker-pycreds	https://github.com/shin-/dockerpy-creds	https://github.com/shin-/dockerpy-creds/blob/master/LICENSE
docopt	https://docopt.org	https://github.com/docopt/docopt/blob/master/LICENSE-MIT
docutils	https://docutils.sourceforge.io	https://docutils.sourceforge.io/COPYING.html
drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields	https://github.com/dbrgn/drf-dynamic-fields/blob/master/LICENSE
DuckDB	https://duckdb.org/	https://github.com/duckdb/duckdb?tab=MIT-1-ov-file#readme
edgembar	https://rutgerslbsr.gitlab.io/fe-toolkit/edgembar/index.html	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
editdistance	https://github.com/roy-ht/editdistance	https://github.com/roy-ht/editdistance/blob/master/LICENSE
eigen	https://eigen.tuxfamily.org/index.php?title=Main_Page	https://eigen.tuxfamily.org/index.php?title=Main_Page#License
einops	https://github.com/arogozhnikov/einops	https://github.com/arogozhnikov/einops/blob/master/LICENSE
einx	https://github.com/fferflo/einx	https://github.com/fferflo/einx/blob/master/LICENSE
entrypoints	https://github.com/takluyver/entrypoints	https://github.com/takluyver/entrypoints/blob/master/LICENSE
errors	https://github.com/pkg/errors	https://github.com/pkg/errors/blob/master/LICENSE

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Name of Project	Website	License URL
eslint-plugin	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile	https://foss.heptapod.net/openpyxl/et_xmlfile/-/blob/branch/default/LICENCE.rst
exceptiongroup	https://github.com/agronholm/exceptiongroup	https://github.com/agronholm/exceptiongroup/blob/main/LICENSE
execnet	https://execnet.readthedocs.io/en/latest/	https://github.com/pytest-dev/execnet/blob/master/LICENSE
executing	https://github.com/alexmojaki/executing	https://github.com/alexmojaki/executing/blob/master/LICENSE.txt
expat	https://libexpat.github.io	https://github.com/libexpat/libexpat/blob/master/expat/COPYING
fairscale	https://github.com/facebookresearch/fairscale	https://github.com/facebookresearch/fairscale/blob/main/LICENSE
fairseq	https://github.com/pytorch/fairseq	https://github.com/facebookresearch/fairseq/blob/main/LICENSE
fastjsonschema	https://github.com/horejsek/python-fastjsonschem	https://github.com/horejsek/python-fastjsonschem/blob/master/LICENSE
fastrlock	https://github.com/scoder/fastrlock	https://github.com/scoder/fastrlock/blob/master/LICENSE
fftw	https://www.fftw.org	commercial license

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Name of Project	Website	License URL
filebuffer	https://github.com/mattetti/filebuffer	https://github.com/mattetti/filebuffer/blob/master/LICENSE
filelock	https://py-filelock.readthedocs.io/en/latest/index.html	https://github.com/tox-dev/py-filelock/blob/main/LICENSE
finufft	https://github.com/flatironinstitute/finufft	https://github.com/flatironinstitute/finufft/blob/master/LICENSE
Flask	https://flask.palletsprojects.com/en/2.1.x/	https://flask.palletsprojects.com/en/2.1.x/license/
flatbuffers	https://google.github.io/flatbuffers/	https://github.com/google/flatbuffers/blob/master/LICENSE.txt
flexcache	https://github.com/hgrecco/flexcache	https://github.com/hgrecco/flexcache/blob/main/LICENSE
flexparser	https://github.com/hgrecco/flexparser	https://github.com/hgrecco/flexparser/blob/main/LICENSE
flit-core	https://github.com/pypa/flit	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
FLTK	https://www.fltk.org/index.php	https://www.fltk.org/COPYING.php
fmt	https://fmt.dev/latest/index.html	https://github.com/fmtlib/fmt/blob/master/LICENSE.rst
font-awesome	https://github.com/FortAwesome/Font-Awesome	https://github.com/FortAwesome/Font-Awesome
font-ttf-dejavu-sans-mono	https://dejavu-fonts.github.io	https://dejavu-fonts.github.io/License.html
font-ttf-inconsolata	https://fonts.google.com/specimen/Inconsolata	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL

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Name of Project	Website	License URL
font-ttf-source-code-pro	https://fonts.google.com/specimen/Source+Code+Pro	https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL
font-ttf-ubuntu	https://fonts.google.com/specimen/Ubuntu	https://ubuntu.com/legal/font-licence
fontconfig	https://www.freedesktop.org/wiki/Software/fontconfig/	https://gitlab.freedesktop.org/fontconfig/fontconfig/-/blob/main/COPYING
fonts-conda-ecosystem	https://anaconda.org/conda-forge/fonts-conda-ecosyster	https://docs.conda.io/en/latest/license.html
fonts-conda-forge	https://anaconda.org/conda-forge/fonts-conda-forge/	https://creativecommons.org/licenses/by/4.0/
fonttools	https://github.com/fonttools/fonttools	https://github.com/fonttools/fonttools/blob/main/LICENSE
forcebalance	https://simtk.org/home/forcebalance OR https://github.com/leeping/forcebalance	https://github.com/leeping/forcebalance/blob/master/LICENSE
fqdn	https://github.com/ypcrts/fqdn	https://github.com/ypcrts/fqdn?tab=MPL-2.0-1-ov-file#readme
freetype	https://freetype.org	https://freetype.org/license.html
freetype-py	https://github.com/rougier/freetype-py	https://github.com/rougier/freetype-py?tab=License-1-ov-file#readme
fribidi	https://github.com/fribidi/fribidi	https://github.com/fribidi/fribidi/blob/master/COPYING
frozendict	https://github.com/Marco-Sulla/python-frozendict	https://github.com/Marco-Sulla/python-frozendict/blob/master/LICENSE.txt
frozenlist	https://github.com/aio-libs/frozenlist	https://github.com/aio-libs/frozenlist/blob/master/LICENSE

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Name of Project	Website	License URL
fsmlite	https://github.com/tkem/fsmlite	https://github.com/tkem/fsmlite/blob/master/LICENSE
fsspec	https://github.com/fsspec/filesystem_spec	https://github.com/fsspec/filesystem_spec/blob/master/LICENSE
funcy	https://github.com/Suor/funcy	https://github.com/Suor/funcy/blob/master/LICENSE
gast	https://github.com/serge-sans-paille/gast/	https://github.com/serge-sans-paille/gast/blob/master/LICENSE
gau2grid	https://github.com/dgasmith/gau2grid	https://github.com/dgasmith/gau2grid/blob/master/LICENSE
gax-go	https://github.com/googleapis/gax-go/v2	https://github.com/googleapis/gax-go/blob/main/LICENSE
gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf	https://gitlab.gnome.org/GNOME/gdk-pixbuf/-/blob/master/COPYING
gemmi	https://gemmi.readthedocs.io/en/latest/	https://github.com/project-gemmi/gemmi/blob/master/LICENSE.txt
genproto	https://google.golang.org/genproto/googleapis	https://github.com/googleapis/go-genproto/blob/main/LICENSE
geometric	https://openbase.com/python/geometric	https://openbase.com/python/geometric
giflib	https://giflib.sourceforge.net	https://github.com/mirrorer/giflib/blob/master/COPYING
gitdb	https://github.com/gitpython-developers/gitdb	https://github.com/gitpython-developers/gitdb/blob/master/LICENSE
GitPython	https://github.com/gitpython-developers/GitPython	https://github.com/gitpython-developers/GitPython/blob/main/LICENSE

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Name of Project	Website	License URL
glib	https://docs.gtk.org/glib/	https://gitlab.gnome.org/GNOME/glib/-/blob/main/LICENSES/LGPL-2.1-or-later.txt
GLM Library	https://github.com/g-truc/glm	https://github.com/g-truc/glm/blob/master/manual.md#section0
gls	https://github.com/jtolds/gls	https://github.com/jtolds/gls/blob/master/LICENSE
gmpy2	https://github.com/aleaxit/gmpy	https://github.com/gmpy2/gmpy2/blob/master/COPYING.LESSER
go-cleanhttp	https://github.com/hashicorp/go-cleanhttp	https://github.com/hashicorp/go-cleanhttp/blob/master/LICENSE
go-connections	https://github.com/docker/go-connections	https://github.com/docker/go-connections/blob/master/LICENSE
go-cpio	https://github.com/cavaliercoder/go-cpio	https://github.com/cavaliercoder/go-cpio/blob/master/LICENSE
go-getter	https://github.com/hashicorp/go-getter	https://github.com/hashicorp/go-getter/blob/master/LICENSE
go-homedir	https://github.com/mitchellh/go-homedir	https://github.com/mitchellh/go-homedir/blob/master/LICENSE
go-ini	https://github.com/go-ini/ini	https://github.com/go-ini/ini/blob/master/LICENSE
go-jmespath	https://github.com/jmespath/go-jmespath	https://github.com/jmespath/go-jmespath/blob/master/LICENSE

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Name of Project	Website	License URL
go-junit-report	https://github.com/jstemmer/go-junit-report	https://github.com/jstemmer/go-junit-report/blob/master/LICENSE
go-netrc	https://github.com/bgentry/go-netrc/netrc	https://github.com/bgentry/go-netrc/blob/master/LICENSE
go-ole	https://github.com/go-ole/go-ole	https://github.com/go-ole/go-ole/blob/master/LICENSE
go-pg	https://github.com/go-pg/pg	https://github.com/go-pg/pg/blob/master/LICENSE
go-redis	https://github.com/go-redis/redis/v8	https://github.com/go-redis/redis/blob/master/LICENSE
go-rendezvous	https://github.com/dgryski/go-rendezvous	https://github.com/dgryski/go-rendezvous/blob/master/LICENSE
go-safetemp	https://github.com/hashicorp/go-safetemp	https://github.com/hashicorp/go-safetemp/blob/master/LICENSE
go-sysconf	https://github.com/tklauser/go-sysconf	https://github.com/tklauser/go-sysconf/blob/master/LICENSE
go-testing-interface	https://github.com/mitchellh/go-testing-interface	https://github.com/mitchellh/go-testing-interface/blob/master/LICENSE
go-units	https://github.com/docker/go-units	https://github.com/docker/go-units/blob/master/LICENSE
go-version	https://github.com/hashicorp/go-version	https://github.com/hashicorp/go-version/blob/master/LICENSE
go-zglob	https://github.com/mattn/go-zglob	https://github.com/mattn/go-zglob/blob/master/LICENSE

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Name of Project	Website	License URL
go.opencensus	https://go.opencensus.io	https://github.com/census-instrumentatio opencensus-go/blob/master/LICENSE
gobrake.v2	https://gopkg.in/airbrake/gobrake.v2	https://github.com/airbrake/gobrake/blob/v2.0.9/LICENSE
goconvey	https://github.com/smartystreets/goconvey	https://github.com/smartystreets/goconvey/blob/master/LICENSE.md
golden-layout	https://github.com/deepstreamIO/golden-layout	https://github.com/deepstreamIO/golden-layout/raw/master/LICENSE
google-auth	https://google-auth.readthedocs.io/en/master/	https://github.com/GoogleCloudPlatform google-auth-library-p blob/master/LICENSE
google-auth-oauthlib	https://github.com/googleapis/google-auth-library-p	https://github.com/googleapis/google-auth-library-p blob/main/LICENSE
google-cloud-go	https://cloud.google.com/go	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-cloud-go/storage	https://cloud.google.com/go/storage	https://github.com/googleapis/google-cloud-go/blob/main/LICENSE
google-pasta	https://github.com/google/pasta	https://github.com/google/pasta/blob/master/LICENSE
google.golang.org/api	https://google.golang.org/api	https://github.com/googleapis/google-api-go-client/blob/main/LICENSE
gopsutil	https://github.com/shirou/gopsutil	https://github.com/shirou/gopsutil/blob/master/LICENSE

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Name of Project	Website	License URL
gorilla websocket	https://github.com/gorilla/websocket	https://github.com/gorilla/websocket/blob/master/LICENSE
gpytorch	https://gpytorch.ai	https://github.com/cornellius-gp/gpytorch?tab=MIT-1-ov-file#readme
graphite2	https://github.com/silnrsi/graphite	https://github.com/silnrsi/graphite/blob/master/LICENSE
graphviz	https://graphviz.org/	https://graphviz.org/license/
greenlet	https://greenlet.readthedocs.io/en/latest/	https://github.com/python-greenlet/greenlet/blob/master/LICENSE
groupcache	https://github.com/golang/groupcache	https://github.com/golang/groupcache/blob/master/LICENSE
grpc	https://google.golang.org/grpc	https://github.com/grpc/grpc-go/blob/master/LICENSE
grpc-cpp	https://github.com/grpc/grpc	https://github.com/grpc/grpc/blob/master/LICENSE
grpcio	https://github.com/grpc/grpc.io/blob/main/LICENSE	https://github.com/grpc/grpc.io/blob/main/LICENSE
gtk2	https://gitlab.gnome.org/GNOME/gtk	https://gitlab.gnome.org/GNOME/gtk/-/blob/main/COPYING
gts	https://sourceforge.net/projects/gts/	https://www.gnu.org/licenses/lgpl-3.0.html
h11	https://github.com/python-hyper/h11	https://github.com/python-hyper/h11/blob/master/LICENSE.txt
h2	https://github.com/python-hyper/h2	https://github.com/python-hyper/h2?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
h5py	https://www.h5py.org	https://docs.h5py.org/en/stable/licenses.html
harfbuzz	https://github.com/harfbuzz/harfbuzz	https://github.com/harfbuzz/harfbuzz/blob/main/COPYING
hdbscan	https://hdbscan.readthedocs.io/en/latest/	https://github.com/scikit-learn-contrib/hdbscan/blob/master/LICENSE
hdf4	https://www.hdfgroup.org/solutions/hdf4/	https://github.com/HDFGroup/hdf4/blob/master/COPYING
hdf5	https://www.hdfgroup.org/solutions/hdf5/	https://github.com/HDFGroup/hdf5/blob/master/COPYING
he	https://github.com/mathiasbynens/he	https://github.com/mathiasbynens/he/raw/master/LICENSE-MIT.txt
hpack	https://github.com/python-hyper/hpack	https://github.com/python-hyper/hpack?tab=MIT-1-ov-file#readme
html-loader	https://github.com/webpack-contrib/html-loader	https://github.com/webpack-contrib/html-loader/raw/master/LICENSE
html5lib	https://github.com/html5lib/html5lib-python	https://github.com/html5lib/html5lib-python/blob/master/LICENSE
htslib	https://www.htslib.org	https://github.com/samtools/htslib/blob/develop/LICENSE
httpcore	https://www.encode.io/httpcore/	https://github.com/encode/httpcore/blob/master/LICENSE.md
httpx	https://github.com/encode/httpx	https://github.com/encode/httpx/blob/master/LICENSE.md

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Name of Project	Website	License URL
humanize	https://github.com/jmoiron/humanize	https://github.com/jmoiron/humanize/blob/master/LICENCE
hydra-core	https://github.com/facebookresearch/hydra	https://github.com/facebookresearch/hydra/blob/main/LICENSE
hyperframe	https://github.com/python-hyper/hyperframe	https://github.com/python-hyper/hyperframe?tab=MIT-1-ov-file#readme
icu	https://github.com/unicode-org/icu	https://github.com/unicode-org/icu/blob/main/icu4c/LICENSE
idna	https://github.com/kjd/idna	https://github.com/kjd/idna/blob/master/LICENSE.md
ihm	https://github.com/ihmwg/python-ihm	https://github.com/ihmwg/python-ihm/blob/main/LICENSE
imageio	https://github.com/imageio/imageio	https://github.com/imageio/imageio/blob/master/LICENSE
imagesize	https://github.com/shibukawa/imagesize_py	https://github.com/shibukawa/imagesize_py/blob/master/LICENSE.rst
ImmuneBuilder	https://github.com/oxpig/ImmuneBuilder/tree/main	https://github.com/oxpig/ImmuneBuilder/blob/main/LICENSE
importlib-metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE
importlib_metadata	https://github.com/python/importlib_metadata	https://github.com/python/importlib_metadata/blob/main/LICENSE

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Name of Project	Website	License URL
importlib_resources	https://github.com/python/importlib_resources	https://github.com/python/importlib_resources/blob/main/LICENSE
InChI	https://iupac.org/who-we-are/divisions/division-details/inchi/	https://iupac.org/wp-content/uploads/2021/06/iupac-inchi-license_2020.pdf
inflection	https://github.com/jinzhu/inflection	https://github.com/jinzhu/inflection/blob/master/LICENSE
ini.v1	https://gopkg.in/ini.v1	https://github.com/go-ini/ini/blob/v1.66.2/LICENSE
iniconfig	https://github.com/pytest-dev/iniconfig	https://github.com/pytest-dev/iniconfig/blob/main/LICENSE
innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill	https://github.com/dnozay/innersvg-polyfill/raw/master/LICENSE
intel-openmp	https://github.com/hermitcore/libomp_oss	https://github.com/hermitcore/libomp_oss/blob/hermit/LICENSE.txt
ipykernel	https://ipython.org	https://ipython.org
ipython	https://ipython.org	https://github.com/ipython/ipython/blob/master/LICENSE
ipython-genutils	http://ipython.org	https://github.com/ipython/ipython_genutils/blob/master/COPYING.md
ipython_pygments_le	https://github.com/ipython/ipython-pygments-lex	https://github.com/ipython/ipython-pygments-lex blob/main/LICENSE
ipywidgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE

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Name of Project	Website	License URL
isodate	https://github.com/gweis/isodate/	https://github.com/gweis/isodate/blob/master/LICENSE
isoduration	https://github.com/bolsote/isoduration	https://github.com/bolsote/isoduration?tab=ISC-1-ov-file#readme
itsdangerous	https://palletsprojects.com/p/itsdangerous/	https://itsdangerous.palletsprojects.com/en/2.1.x/license/
jax	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxlib	https://github.com/google/jax	https://github.com/google/jax/blob/main/LICENSE
jaxtyping	https://github.com/patrick-kidger/jaxtyping	https://github.com/patrick-kidger/jaxtyping?tab=License-1-ov-file#readme
jedi	https://jedi.readthedocs.io/en/latest/	https://github.com/davidhalter/jedi/blob/master/LICENSE.txt
Jinja2	https://palletsprojects.com/p/jinja/	https://github.com/pallets/jinja/blob/main/LICENSE.rst
jmespath	https://github.com/jmespath/jmespath.py	https://github.com/jmespath/jmespath.py/blob/develop/LICENSE.txt
joblib	https://joblib.readthedocs.io/en/latest/	https://github.com/joblib/joblib/blob/master/LICENSE.txt
jpeg	https://www.ijg.org	https://www.ijg.org/files/README
json5	https://github.com/dpranke/pyjson5	https://github.com/dpranke/pyjson5/blob/main/LICENSE
jsonfield	https://github.com/dmkoch/django-jsonfield/	https://github.com/rpkilby/jsonfield/blob/master/LICENSE

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Name of Project	Website	License URL
jsonpatch	https://github.com/stefankoegl/python-json-patch	https://github.com/stefankoegl/python-json-patch/blob/master/LICENSE
jsonpickle	https://github.com/jsonpickle/jsonpickle	https://github.com/jsonpickle/jsonpickle/blob/main/LICENSE
jsonpointer	https://github.com/stefankoegl/python-json-pointer	https://github.com/stefankoegl/python-json-pointer/blob/master/LICENSE.txt
jsonschema	https://github.com/python-jsonschema/jsonschema	https://github.com/python-jsonschema/jsonschema/blob/master/COPYING
jsonschema-specifications	https://github.com/python-jsonschema/jsonschema-specificat	https://github.com/python-jsonschema/jsonschema-specificat blob/main/COPYING
jstat	https://github.com/jstat/jstat	https://www.opensource.org/licenses/mit-license.php
jupyter-client	https://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/COPYING.md
jupyter-core	https://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/COPYING.md
jupyter-events	https://github.com/jupyter/jupyter_events	https://github.com/jupyter/jupyter_events/blob/main/LICENSE
jupyter-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp	https://github.com/jupyter-lsp/jupyterlab-lsp
jupyter-serverhttp://jupyter.or	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE	
jupyter_client	http://jupyter.org	https://github.com/jupyter/jupyter_client/blob/main/LICENSE

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Name of Project	Website	License URL
jupyter_core	http://jupyter.org	https://github.com/jupyter/jupyter_core/blob/master/LICENSE
jupyter_server	https://github.com/jupyter-server/jupyter_server	https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE
jupyter_server_termin	https://github.com/jupyter-server/jupyter_server_terminals	https://github.com/jupyter-server/jupyter_server_terminals/blob/main/LICENSE
jupyterlab	https://github.com/jupyterlab/jupyterlab	https://github.com/jupyterlab/jupyterlab/blob/main/LICENSE
jupyterlab-pygments	http://jupyter.org	https://github.com/jupyterlab/jupyterlab_pygments/blob/main/LICENSE
jupyterlab-widgets	http://jupyter.org	https://github.com/jupyter-widgets/ipywidgets/blob/master/LICENSE
jupyter-lab_pygments	https://github.com/jupyterlab/jupyterlab_pygments	https://github.com/jupyterlab/jupyterlab_pygments?tab=BSD-3-Clause-1-ov-file#readme
jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server	https://github.com/jupyterlab/jupyterlab_server/blob/main/LICENSE
jupyterlab_widgets	https://github.com/jupyter-widgets/ipywidgets	https://github.com/jupyter-widgets/ipywidgets?tab=BSD-3-Clause-1-ov-file#readme
kaleido	https://github.com/plotly/Kaleido	https://github.com/plotly/Kaleido/blob/master/LICENSE.txt
keras	https://github.com/keras-team/keras	https://github.com/keras-team/keras/blob/master/LICENSE

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Name of Project	Website	License URL
Keras-Preprocessing	https://github.com/keras-team/keras-preprocessing	https://github.com/keras-team/keras-preprocessing/blob/master/LICENSE
keras-tuner	https://github.com/keras-team/keras-tuner	https://github.com/keras-team/keras-tuner/blob/master/LICENSE
keyring	https://github.com/jaraco/keyring	https://github.com/jaraco/keyring/blob/main/LICENSE
keyutils	https://github.com/sassoftware/python-keyutils	https://github.com/sassoftware/python-keyutils/blob/master/LICENSE
kiwisolver	https://kiwisolver.readthedocs.io/en/latest/	https://github.com/nucleic/kiwi/blob/main/LICENSE
kombu	https://kombu.readthedocs.io	https://github.com/celery/kombu/blob/master/LICENSE
krb5	https://web.mit.edu/kerberos/	https://github.com/krb5/krb5/blob/master/src/lib/gssapi/LICENSE
kt-legacy	https://github.com/haifeng-jin/kt-legacy	https://github.com/haifeng-jin/kt-legacy/blob/main/LICENSE
lark	https://github.com/lark-parser/lark	https://github.com/lark-parser/lark?tab=MIT-1-ov-file#readme
lazy_loader	https://github.com/scientific-python/lazy_loader	https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md
lcms2	https://www.littlecms.com	https://github.com/sk1project/python-lcms2/blob/master/LICENSE
legacy-cgi	https://github.com/jackrosenthal/legacy-cgi	https://github.com/jackrosenthal/legacy-cgi?tab=License-1-ov-file#readme

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Name of Project	Website	License URL
lerc	https://github.com/Esri/lerc	https://github.com/Esri/lerc/blob/master/LICENSE
libarchive	http://www.libarchive.org	https://raw.githubusercontent.com/libarchive/libarchive/master/COPYING
libblas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
libbrotlicommon	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlidec	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libbrotlienc	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
libcblas	https://anaconda.org/conda-forge/libcblas	N/A
libclang	https://github.com/sighingnow/libclang	https://github.com/sighingnow/libclang/blob/master/LICENSE.TXT
libcurl	https://curl.se/libcurl/	https://curl.se/docs/copyright.html
libcxx	https://github.com/llvm-mirror/libcxx	https://github.com/llvm-mirror/libcxx/blob/master/LICENSE.TXT
libdb	https://www.oracle.com/technology/software/products/berkeley-db/index.html	https://github.com/berkeleydb/libdb/blob/master/LEGAL
libdeflate	https://github.com/ebiggers/libdeflate	https://github.com/ebiggers/libdeflate/blob/master/COPYING
libedit	https://thrysoee.dk/editline/	http://www.netbsd.org/Goals/redistribution.html
libev	https://software.schmorp.de/pkg/libev.html	https://software.schmorp.de/pkg/libev.html

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Name of Project	Website	License URL
libexpat	https://libexpat.github.io/	https://github.com/libexpat/libexpat?tab=MIT-1-ov-file#readme
libffi	https://github.com/libffi/libffi	https://github.com/libffi/libffi/blob/master/LICENSE
libgcc	https://gcc.gnu.org/onlinedocs/gccint/Libgcc.html	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libgcrypt	https://gnupg.org/software/index.html	https://git.gnupg.org/cgi-bin/gitweb.cgi?p=libgcrypt.git;a=blob;f=COPYING.LIB;hb=HEAD
libgd	https://libgd.github.io	https://libgd.github.io/manuals/2.2.1/files/license-txt.html
libglib	https://github.com/PolMine/libglib	https://github.com/PolMine/libglib/blob/master/include/glib-2.0/glib.h
libiconv	https://www.gnu.org/software/libiconv/	https://www.gnu.org/software/libiconv/#downloading
libint	https://tinyurl.com/yvw97wbw	https://tinyurl.com/yvw97wbw
liblapack	http://www.netlib.org/lapack/	https://www.netlib.org/lapack/LICENSE.txt
liblapacke	https://anaconda.org/conda-forge/liblapacke	https://www.netlib.org/lapack/LICENSE.txt
liblzma	https://tukaani.org/xz/	https://git.tukaani.org/?p=xz.git;a=blob;f=COPYING.0BSD
libmamba	https://medium.com/@QuantStack/open-software-packag	https://github.com/mamba-org/mamba/blob/main/LICENSE

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Name of Project	Website	License URL
libmambapy	https://www.anaconda.com/blog/a-faster-conda-for-a-g	https://github.com/conda/conda-libmamba-solv blob/main/LICENSE
libnetcdf	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
libnghttp2	https://github.com/nghttp2/nghttp2	https://github.com/nghttp2/nghttp2/blob/master/COPYING
libnsl	https://github.com/thkukuk/libnsl	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html
libopenblas	https://www.openblas.net/	https://github.com/xianyi/OpenBLAS/blob/develop/LICENSE
libpng	https://www.libpng.org/pub/png/libpng.html	https://www.libpng.org/pub/png/src/libpng-LICENSE.txt
libpq	https://www.postgresql.org/	https://www.postgresql.org/about/licence/
librsvg	https://gitlab.gnome.org/GNOME/librsvg	https://gitlab.gnome.org/GNOME/librsvg/-/blob/main/COPYING.LIB
libsolv	https://github.com/openSUSE/libsolv	https://github.com/openSUSE/libsolv/blob/master/LICENSE.BSD
libsqlite	https://github.com/mackyle/sqlite	https://github.com/mackyle/sqlite?tab=License-1-ov-file#readme
libssh2	https://github.com/libssh2/libssh2	https://github.com/libssh2/libssh2/blob/master/COPYING
libstdcxx	https://gcc.gnu.org/	https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html

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Name of Project	Website	License URL
libtiff	https://www.libtiff.org/	https://www.libtiff.org/misc.html
libtrust	https://github.com/docker/libtrust	https://github.com/docker/libtrust/blob/master/LICENSE
libuuid	https://sourceforge.net/projects/libuuid/	https://sourceforge.net/p/libuuid/code/ci/master/tree/COPYING
libuv	https://github.com/libuv/libuv	https://github.com/libuv/libuv/blob/v1.x/LICENSE
libwebp	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libwebp-base	https://chromium.googlesource.com/?format=HTML	https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE
libxc	https://www.tddft.org/programs/libxc/	https://gitlab.com/libxc/libxc/-/blob/master/COPYING
libxcb	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-libxcb/blob/master/COPYING
libxcrypt	https://github.com/besser82/libxcrypt	https://github.com/besser82/libxcrypt?tab=LGPL-2.1-1-ov-file#readme
libxml2	https://git.gnome.org/browse/libxml2/	https://gitlab.gnome.org/GNOME/libxml2/-/blob/master/Copyright
libxmlsec1	https://github.com/lsh123/xmlsec	https://github.com/lsh123/xmlsec/blob/master/README
libxslt	https://gitlab.gnome.org/GNOME/libxslt/-/wikis/home	https://gitlab.gnome.org/GNOME/libxslt/-/blob/master/Copyright

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Name of Project	Website	License URL
libzlib	https://zlib.net	https://zlib.net/zlib_license.html
lightning-utilities	https://github.com/Lightning-AI/utilities	https://github.com/Lightning-AI/utilities?tab=Apache-2.0-1-ov-file#readme
lime	https://github.com/marcotcr/lime	https://github.com/marcotcr/lime/blob/master/LICENSE
linear-operator	https://github.com/cornellius-gp/linear_operator	https://github.com/cornellius-gp/linear_operator?tab=MIT-1-ov-file#readme
lit	http://llvm.org	https://releases.llvm.org/14.0.0/LICENSE.TXT
llvm-openmp	https://github.com/llvm-mirror/openmp	https://github.com/llvm-mirror/openmp/blob/master/LICENSE.txt
llvmlite	http://llvmlite.readthedocs.io	https://github.com/numba/llvmlite/blob/main/LICENSE
loader-utils	https://github.com/webpack/loader-utils	https://github.com/webpack/loader-utils/raw/master/LICENSE
logistro	https://github.com/geopozo/logistro	https://github.com/geopozo/logistro?tab=MIT-1-ov-file#readme
logomaker	https://logomaker.readthedocs.io/en/latest/	https://github.com/jbkinney/logomaker/blob/master/LICENSE
logrus	https://github.com/sirupsen/logrus	https://github.com/sirupsen/logrus/blob/master/LICENSE
logrus-airbrake-hook.v2	https://gopkg.in/gemnasium/logrus-airbrake-hook.v2	https://github.com/gemnasium/logrus-airbrake-hook/blob/v2.1.2/LICENSE
lxml	https://lxml.de	https://lxml.de/index.html#license

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Name of Project	Website	License URL
lz4-c	https://www.lz4.org/	https://github.com/lz4/lz4/blob/dev/LICENSE
lzo	https://www.oberhumer.com/opensource/lzo/	https://www.oberhumer.com/opensource/gpl.html
mamba	https://github.com/mamba-org/mamba	https://github.com/mamba-org/mamba?tab=BSD-3-Clause-1-ov-f readme
markdown	https://github.com/evilstreak/markdown-js	https://www.opensource.org/licenses/mit-license.php
markdown-it-py	https://github.com/executablebooks/markdown-it-py	https://github.com/executablebooks/markdown-it-py/blob/master/LICENSE
markupsafe	https://github.com/pallets/markupsafe/tree/main/src/markupsafe	https://github.com/pallets/markupsafe/tree/main?tab=BSD-3-Clause-1-ov-f
MarkupSafe	https://palletsprojects.com/p/markupsafe/	https://github.com/pallets/markupsafe/blob/main/LICENSE.rst
mashumaro	https://github.com/Fatal1ty/mashumaro	https://github.com/Fatal1ty/mashumaro
matplotlib	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-base	https://matplotlib.org	https://matplotlib.org/stable/users/project/license.html
matplotlib-inline	https://github.com/ipython/matplotlib-inline	https://github.com/ipython/matplotlib-inline/blob/master/LICENSE
mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib/blob/main/LICENSE

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Name of Project	Website	License URL
mda_xdrlib	https://github.com/MDAnalysis/mda-xdrlib	https://github.com/MDAnalysis/mda-xdrlib?tab=License-1-ov-file#readme
mdtraj	https://www.mdtraj.org/	https://www.mdtraj.org/1.9.8.dev0/index.html#license
mdurl	https://github.com/markdown-it/mdurl	https://github.com/markdown-it/mdurl/blob/master/LICENSE
menuinst	https://github.com/conda/menuinst	https://github.com/conda/menuinst/blob/main/LICENSE.txt
mergo	https://github.com/imdario/mergo	https://github.com/imdario/mergo/blob/master/LICENSE
mistune	https://github.com/lepture/mistune	https://github.com/lepture/mistune/blob/master/LICENSE
mkl	https://github.com/rust-math/intel-mkl-src	https://github.com/rust-math/intel-mkl-src/blob/master/License.txt
mkl-fft	https://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft/blob/master/LICENSE.txt
mkl-random	https://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random/blob/master/LICENSE.txt
mkl-service	https://github.com/IntelPython/mkl-service	https://github.com/IntelPython/mkl-service/blob/master/LICENSE.txt
mkl_fft	http://github.com/IntelPython/mkl_fft	https://github.com/IntelPython/mkl_fft?tab=BSD-3-Clause-1-ov-file#readme

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Name of Project	Website	License URL
mkl_random	http://github.com/IntelPython/mkl_random	https://github.com/IntelPython/mkl_random?tab=BSD-3-Clause-1-ov-f readme
ml-dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
ml_dtypes	https://github.com/jax-ml/ml_dtypes	https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE
modelcif	https://github.com/ihmwg/python-modelcif	https://github.com/ihmwg/python-modelcif/blob/main/LICENSE
molecupy	https://molecupy.readthedocs.io/en/latest/	https://github.com/samirelanduk/atomium/blob/master/LICENSE
moment	https://github.com/moment/moment	https://github.com/moment/moment/raw/master/LICENSE
moment-precise-range-plugin	https://github.com/codebox/moment-precise-range	https://github.com/codebox/moment-precise-range raw/master/LICENSE.md
more-itertools	https://github.com/more-itertools/more-itertools	https://github.com/more-itertools/more-itertools/blob/master/LICENSE
mpiplus	https://github.com/choderalab/mpiplus	https://github.com/choderalab/mpiplus/blob/main/LICENSE
mpmath	http://mpmath.org/	https://github.com/mpmath/mpmath/blob/master/LICENSE
mrcfile	https://github.com/ccpem/mrcfile	https://github.com/ccpem/mrcfile/blob/master/LICENSE.txt

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Name of Project	Website	License URL
msgpack	https://msgpack.org/	https://github.com/msgpack/msgpack-python/blob/main/COPYING
multidict	https://github.com/aio-libs/multidict	https://github.com/aio-libs/multidict/blob/master/LICENSE
multierr	https://go.uber.org/multierr	https://github.com/uber-go/multierr/blob/master/LICENSE.txt
multiprocess	https://github.com/uqfoundation/multiprocess	https://github.com/uqfoundation/multiprocess/blob/master/LICENSE
munkres	https://software.clapper.org/munkres/	https://github.com/bmc/munkres/blob/master/LICENSE.md
myesui uuid	https://github.com/myesui/uuid	https://pkg.go.dev/github.com/myesui/uuid?tab=licenses
namex	https://github.com/bcgov/namex	https://github.com/bcgov/namex/blob/main/LICENSE
narwhals	https://github.com/narwhals-dev/narwhals	https://github.com/narwhals-dev/narwhals?tab=MIT-1-ov-file#readme
nbclassic	http://jupyter.org	https://github.com/jupyter/nbclassic/blob/main/LICENSE
nbclient	https://jupyter.org	https://github.com/jupyter/nbclient/blob/main/LICENSE
nbconvert	https://jupyter.org	https://github.com/jupyter/nbconvert/blob/main/LICENSE
nbformat	http://jupyter.org	https://github.com/jupyter/nbformat/blob/main/LICENSE

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Name of Project	Website	License URL
ncurses	https://invisible-island.net/ncurses/	https://invisible-island.net/ncurses/ncurses-license.html
ndfes	https://rutgerslbsr.gitlab.io/fe-toolkit/	https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE
ndindex	https://quansight-labs.github.io/ndindex/	https://github.com/Quansight-Labs/ndindex?tab=MIT-1-ov-file#readme
nest-asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio/blob/master/LICENSE
nest_asyncio	https://github.com/erdewit/nest_asyncio	https://github.com/erdewit/nest_asyncio?tab=BSD-2-Clause-1-ov-f readme
netcdf-fortran	https://www.unidata.ucar.edu/software/netcdf/	https://www.unidata.ucar.edu/software/netcdf/copyright.html
netCDF4	http://github.com/Unidata/netcdf4-python	https://github.com/Unidata/netcdf4-python/blob/master/LICENSE
nettle	https://git.lysator.liu.se/nettle/nettle	https://git.lysator.liu.se/nettle/nettle/-/blob/master/AUTHORS?ref_type=heads
networkx	https://networkx.org	https://github.com/networkx/networkx/blob/main/LICENSE.txt
nfpm	https://github.com/goreleaser/nfpm	https://github.com/goreleaser/nfpm/blob/master/LICENSE.md
ng-tags-input	https://github.com/mbenford/ngTagsInput	https://github.com/mbenford/ngTagsInput
ng-toast	https://github.com/tameraydin/ngToast	https://github.com/tameraydin/ngToast

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Name of Project	Website	License URL
ngdraggable	https://github.com/fatlinesofcode/ngDraggable	https://github.com/fatlinesofcode/ngDraggable/raw/master/LICENSE.txt
ngVue	https://github.com/ngVue/ngVue	https://github.com/ngVue/ngVue/raw/master/LICENSE
nh3	https://nh3.readthedocs.io/en/latest/	https://github.com/messense/nh3/blob/main/LICENSE
nlohmann_json	https://github.com/nlohmann/json	https://github.com/nlohmann/json?tab=MIT-1-ov-file#readme
nlopt	https://nlopt.readthedocs.io/en/latest/NLopt_Python_Reference/	https://nlopt.readthedocs.io/en/latest/NLopt_License_and_Copyright/
nodejs	https://nodejs.org/en/	https://raw.githubusercontent.com/nodejs/node/master/LICENSE
nomkl	https://github.com/conda-forge/nomkl-feedstock	https://github.com/conda-forge/nomkl-feedstock/blob/main/LICENSE.txt
notebook	http://jupyter.org	https://github.com/jupyter/notebook/blob/main/LICENSE
notebook-shim	https://github.com/jupyter/notebook_shim	https://github.com/jupyter/notebook_shim
notebook_shim	http://jupyter.org	https://github.com/jupyter/notebook_shim/blob/main/LICENSE
numba	https://numba.pydata.org	https://github.com/numba/numba/blob/main/LICENSE
numcpus	https://github.com/tklauser/numcpus	https://github.com/tklauser/numcpus/blob/master/LICENSE

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Name of Project	Website	License URL
numexpr	https://github.com/pydata/numexpr	https://github.com/pydata/numexpr/blob/master/LICENSE.txt
numpy	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpy-base	https://numpy.org	https://github.com/numpy/numpy/blob/main/LICENSE.txt
numpydoc	https://numpydoc.readthedocs.io/en/latest/index.html	https://github.com/numpy/numpydoc/blob/main/LICENSE.txt
nvidia-cublas-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cublas-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-cupti-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-nvrtc-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cuda-runtime-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cudnn-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html
nvidia-cudnn-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/deeplearning/cudnn/sla/index.html

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Name of Project	Website	License URL
nvidia-cuEquivariance	https://github.com/NVIDIA/cuEquivariance	https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE
nvidia-cufft-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufft-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cufile-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html#
nvidia-curand-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-curand-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusolver-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparse-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-cusparselt-cu12	https://docs.nvidia.com/cuda/cusparselt/index.html	https://docs.nvidia.com/cuda/cusparselt/license.html
nvidia-ml-py	https://pypi.org/project/nvidia-ml-py/	https://pypi.org/project/nvidia-ml-py/
nvidia-nccl-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nccl-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/hpc-sdk/eula/index.html
nvidia-nvjitlink-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html

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Name of Project	Website	License URL
nvidia-nvshmem-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu11	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
nvidia-nvtx-cu12	https://developer.nvidia.com/cuda-zone	https://docs.nvidia.com/cuda/eula/index.html
Oat++	https://oatpp.io/	https://github.com/oatpp/oatpp/blob/master/LICENSE
oauthlib	https://github.com/oauthlib/oauthlib	https://github.com/oauthlib/oauthlib/blob/master/LICENSE
ocl-icd	https://github.com/OCL-dev/ocl-icd	https://github.com/OCL-dev/ocl-icd/blob/master/COPYING
ocl-icd-system	https://github.com/conda-forge/ocl-icd-system-feedst	https://github.com/conda-forge/ocl-icd-system-feedst blob/main/LICENSE.txt
olefile	https://www.decalage.info/python/olefileio	https://olefile.readthedocs.io/en/latest/License.html
omegaconf	https://github.com/omry/omegaconf	https://github.com/omry/omegaconf/blob/master/LICENSE
OmegaFold	https://github.com/HeliXonProtein/OmegaFold/tree/main	https://github.com/HeliXonProtein/OmegaFold/blob/main/LICENSE
omnicanvas	https://omnicanvas.readthedocs.io/en/latest/	https://github.com/samirelanduk/omnicanvas/blob/master/LICENSE
OpenFF	https://openforcefield.org/	https://github.com/openforcefield/openff-forcefields
openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports	https://github.com/openforcefield/openff-amber-ff-ports blob/main/LICENSE

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Name of Project	Website	License URL
openff-forcefields	https://openforcefield.org	https://github.com/openforcefield/openff-forcefields/blob/master/LICENSE
openff-fragmenter	https://github.com/openforcefield/openff-fragmenter	https://github.com/openforcefield/openff-fragmenter/blob/main/LICENSE
openff-interchange	https://github.com/openforcefield/openff-interchange	https://github.com/openforcefield/openff-interchange/blob/main/LICENSE
openff-models	https://github.com/openforcefield/openff-models	https://github.com/openforcefield/openff-models/blob/main/LICENSE
openff-nagl	https://docs.openforcefield.org/projects/nagl/en/latest/?badge=latest	https://github.com/openforcefield/openff-nagl/blob/main/LICENSE
openff-nagl-models	https://github.com/openforcefield/openff-nagl-models	https://github.com/openforcefield/openff-nagl-models/blob/main/LICENSE
openff-toolkit	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-toolkit-base	https://openforcefield.org	https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE
openff-units	https://github.com/openforcefield/openff-units	https://github.com/openforcefield/openff-units/blob/main/LICENSE
openff-utilities	https://github.com/openforcefield/openff-utilities	https://github.com/openforcefield/openff-utilities/blob/main/LICENSE
openjpeg	https://github.com/uclouvain/openjpeg	https://github.com/uclouvain/openjpeg/blob/master/LICENSE

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Name of Project	Website	License URL
openldap	https://www.openldap.org/software/repo.html	https://git.openldap.org/openldap/openldap/-/blob/master/LICENSE
OpenMM	https://openmm.org	https://docs.openmm.org/7.1.0/userguide/library.html#license
openmmtools	https://github.com/choderalab/openmmtools	https://github.com/choderalab/openmmtools/blob/main/LICENSE
openmoltools	https://github.com/choderalab/openmoltools	https://github.com/choderalab/openmoltools/blob/master/LICENSE
openpyxl	https://openpyxl.readthedocs.io/en/stable/	https://foss.heptapod.net/openpyxl/openpyxl/-/blob/branch/3.0/LICENCE.rst
openssl	https://www.openssl.org	https://github.com/openssl/openssl/blob/master/LICENSE.txt
opt-einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/master/LICENSE
opt_einsum	https://github.com/dgasmith/opt_einsum	https://github.com/dgasmith/opt_einsum/blob/main/LICENSE
OptKing	https://github.com/psi-rking/optking	https://github.com/psi-rking/optking/blob/master/LICENSE
optree	https://optree.readthedocs.io/en/latest/	https://github.com/metaopt/optree/blob/main/LICENSE
oscrypto	https://github.com/wbond/oscrypto	https://github.com/wbond/oscrypto/blob/master/LICENSE
overrides	https://github.com/mkorpela/overrides	https://github.com/mkorpela/overrides/blob/main/LICENSE

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Name of Project	Website	License URL
packaging	https://github.com/pypa/packaging	https://github.com/pypa/packaging/blob/main/LICENSE
packmol	https://leandro.iqm.unicamp.br/m3g/packmol/home.shtml	https://github.com/m3g/packmol/blob/master/LICENSE
packmol_memgen	http://cpclab.uni-duesseldorf.de/	https://gitlab.com/cbjh/memgen/py-memgen/-/blob/main/LICENSE
pandas	https://pandas.pydata.org	https://github.com/pandas-dev/pandas/blob/main/LICENSE
pandocfilters	http://github.com/jgm/pandocfilters	https://github.com/jgm/pandocfilters/blob/master/LICENSE
panedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pango	https://pango.gnome.org	https://gitlab.gnome.org/GNOME/pango/-/blob/main/COPYING
ParmEd	https://parmed.github.io/ParmEd/html/index.html	https://github.com/ParmEd/ParmEd#license
parser	https://github.com/typescript-eslint/typescript-eslint	https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE
parso	https://parso.readthedocs.io/en/latest/	https://github.com/davidhalter/parso/blob/master/LICENSE.txt
pathos	https://github.com/uqfoundation/pathos	https://github.com/uqfoundation/pathos/blob/master/LICENSE
patsy	https://patsy.readthedocs.io/en/latest/	https://github.com/pydata/patsy/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pbkdf2	https://golang.org/x/crypto/pbkdf2	https://cs.opensource.google/go/x/crypto/+/master:LICENSE
pbr	https://docs.openstack.org/pbr/latest/	https://opendev.org/openstack/pbr/src/branch/master/LICENSE
pcmsolver	https://pcmsolver.readthedocs.io/en/stable/	https://github.com/PCMSolver/pcmsolver/blob/master/LICENSE
pcre	https://www.pcre.org	https://www.pcre.org/licence.txt
pcre2	https://www.pcre.org	https://github.com/PCRE2Project/pcre2/blob/master/LICENCE
pdb4amber	https://github.com/Amber-MD/pdb4amber	https://github.com/Amber-MD/pdb4amber/blob/master/LICENSE
pdbfixer	https://github.com/openmm/pdbfixer	https://github.com/openmm/pdbfixer/blob/master/LICENSE
pexpect	https://pexpect.readthedocs.io/	https://github.com/pexpect/pexpect/blob/master/LICENSE
pgconn	https://github.com/jackc/pgconn	https://github.com/jackc/pgconn/blob/master/LICENSE
pgio	https://github.com/jackc/pgio	https://github.com/jackc/pgio/blob/master/LICENSE
pgpassfile	https://github.com/jackc/pgpassfile	https://github.com/jackc/pgpassfile/blob/master/LICENSE
pgproto3	https://github.com/jackc/pgproto3/v2	https://github.com/jackc/pgproto3/blob/master/LICENSE
pgtype	https://github.com/jackc/pgtype	https://github.com/jackc/pgtype/blob/master/LICENSE
pgx	https://github.com/jackc/pgx/v4	https://github.com/jackc/pgx/blob/v4.0.1/LICENSE

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Name of Project	Website	License URL
phonopy	https://github.com/phonopy/phono3py	https://github.com/phonopy/phono3py/blob/develop/LICENSE
pickleshare	https://github.com/pickleshare/pickleshare	https://github.com/pickleshare/pickleshare/blob/master/LICENSE
Pillow	https://python-pillow.org	https://github.com/python-pillow/Pillow/blob/main/LICENSE
Pint	https://pint.readthedocs.io/en/stable/	https://github.com/hgrecco/pint/blob/master/LICENSE
pip	https://pip.pypa.io/	https://github.com/pypa/pip/blob/main/LICENSE.txt
pip-licenses	https://github.com/raimon49/pip-licenses	https://github.com/raimon49/pip-licenses/blob/master/LICENSE
pixman	https://pixman.org	https://cgit.freedesktop.org/pixman/tree/COPYING
pkginfo	https://launchpad.net/pkginfo	https://bazaar.launchpad.net/~tseaver/pkginfo/trunk/view/head:/LICENSE.txt
pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
pkgutil_resolve_name	https://github.com/graingert/pkgutil-resolve-name	https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme
platformdirs	https://github.com/platformdirs/platformdirs	https://github.com/platformdirs/platformdirs/blob/main/LICENSE

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Name of Project	Website	License URL
plotly	https://plotly.com/python/	https://github.com/plotly/plotly.py/blob/master/LICENSE.txt
plotly-orca	https://github.com/plotly/orca	https://github.com/plotly/orca/blob/master/LICENSE
plotly.js	https://github.com/plotly/plotly.js	https://github.com/plotly/plotly.js/raw/master/LICENSE
pluggy	https://pluggy.readthedocs.io/en/stable/index.html	https://github.com/pytest-dev/pluggy/blob/main/LICENSE
pooch	https://github.com/fatiando/pooch	https://github.com/fatiando/pooch/blob/main/LICENSE.txt
portalocker	https://github.com/WoLpH/portalocker	https://github.com/wolph/portalocker/blob/develop/LICENSE
pox	https://github.com/uqfoundation/pox	https://github.com/uqfoundation/pox/blob/master/LICENSE
ppft	https://github.com/uqfoundation/ppft	https://github.com/uqfoundation/ppft/blob/master/LICENSE
pq	https://github.com/lib/pq	https://github.com/lib/pq/blob/master/LICENSE.md
ProDy	http://www.csb.pitt.edu/ProDy	https://github.com/prody/ProDy/blob/master/LICENSE.rst
prometheus-client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prometheus_client	https://github.com/prometheus/client_python	https://github.com/prometheus/client_python/blob/master/LICENSE
prompt-toolkit	https://python-prompt-toolkit.readthedocs.io/en/stable/	https://github.com/prompt-toolkit/python-prompt-toolkit/blob/master/LICENSE

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Name of Project	Website	License URL
prompt_toolkit	https://github.com/prompt-toolkit/python-prompt-toolki	https://github.com/prompt-toolkit/python-prompt-toolki tab=BSD-3-Clause-1-ov-f readme
propcache	https://github.com/aio-libs/propcache	https://github.com/aio-libs/propcache?tab=Apache-2.0-1-ov-file#readme
protobuf	https://google.golang.org/protobuf	https://github.com/protocolbuffers/protobuf-go/blob/master/LICENSE
psi4	https://psicode.org	https://github.com/psi4/psi4/blob/master/COPYING.LESSER
psutil	https://psutil.readthedocs.io/en/latest/	https://github.com/giampaolo/psutil/blob/master/LICENSE
psycopg2	https://psycopg.org/	https://github.com/psycopg/psycopg2/blob/master/LICENSE
PTable	https://github.com/kxxoling/PTable	https://github.com/kxxoling/PTable/blob/master/COPYING
pthread-stubs	https://xcb.freedesktop.org	https://github.com/freedesktop/xcb-pthread-stubs/blob/master/COPYING
ptyprocess	https://ptyprocess.readthedocs.io/en/latest/	https://github.com/pexpect/ptyprocess/blob/master/LICENSE
pure-eval	http://github.com/alexmojaki/pure_eval	http://github.com/alexmojaki/pure_eval/blob/master/LICENSE.txt
pure_eval	http://github.com/alexmojaki/pure_eval	https://github.com/alexmojaki/pure_eval?tab=MIT-1-ov-file#readme

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Name of Project	Website	License URL
py	https://py.readthedocs.io/en/latest/	https://github.com/pytest-dev/py/blob/master/LICENSE
py-cpuinfo	https://github.com/workhorsy/py-cpuinfo	https://github.com/workhorsy/py-cpuinfo/blob/master/LICENSE
pyasn1	https://github.com/etingof/pyasn1	https://github.com/etingof/pyasn1/blob/master/LICENSE.rst
pyasn1-modules	https://github.com/etingof/pyasn1-modules	https://github.com/etingof/pyasn1-modules/blob/master/LICENSE.txt
pyasn1_modules	https://pyasn1.readthedocs.io/en/latest/contents.html	https://github.com/pyasn1/pyasn1-modules?tab=BSD-2-Clause-1-ov-file#readme
pybind11	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11-abi	https://github.com/pybind/pybind11	https://github.com/pybind/pybind11/blob/master/LICENSE
pybind11_global	http://pybind11.readthedocs.io/en/stable/	https://github.com/pybind/pybind11/blob/master/LICENSE
pycairo	https://pycairo.readthedocs.io/en/latest/index.html	https://github.com/pygobject/pycairo/blob/master/COPYING
pycosat	https://github.com/conda/pycosat	https://github.com/conda/pycosat/blob/main/LICENSE
pycparser	https://github.com/eliben/pycparser	https://github.com/eliben/pycparser/blob/master/LICENSE
pydantic	https://pydantic-docs.helpmanual.io	https://github.com/samuelcolvin/pydantic/blob/master/LICENSE

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Name of Project	Website	License URL
pydantic-core	https://github.com/pydantic/pydantic-core	https://github.com/pydantic/pydantic-core
pyedr	https://github.com/MDAnalysis/panedr	https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt
pyEMMA	http://github.com/markovmodel/PyEMMA	https://github.com/markovmodel/PyEMMA/blob/devel/LICENSE.txt
Pygments	https://pygments.org	https://github.com/pygments/pygments/blob/master/LICENSE
pygments	https://pygments.org/	https://github.com/pygments/pygments?tab=BSD-2-Clause-1-ov-file#readme
pygraphviz	https://pygraphviz.github.io	https://github.com/pygraphviz/pygraphviz/blob/main/LICENSE
pygtop	https://pygtop.readthedocs.io/en/latest/	https://github.com/samirelanduk/pygtop/blob/master/LICENSE
pyHanko	https://github.com/MatthiasValvekens/pyHanko	https://github.com/MatthiasValvekens/pyHanko/blob/master/LICENSE
pyhanko-certvalidator	https://github.com/MatthiasValvekens/certvalidator	https://github.com/MatthiasValvekens/certvalidator/blob/master/LICENSE
PyJWT	https://github.com/jpadilla/pyjwt	https://github.com/jpadilla/pyjwt/blob/master/LICENSE
pymbar	https://pymbar.org	https://github.com/choderalab/pymbar/blob/master/LICENSE
pynvml	https://github.com/gpuopenanalytics/pynvml	https://github.com/gpuopenanalytics/pynvml/blob/master/LICENSE.txt

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Name of Project	Website	License URL
pyOpenSSL	https://pyopenssl.org/	https://github.com/pyca/pyopenssl/blob/main/LICENSE
pyparsing	https://pyparsing-docs.readthedocs.io/en/latest/	https://github.com/pyparsing/pyparsing/blob/master/LICENSE
PyPDF3	https://github.com/sfneal/PyPDF3	https://github.com/sfneal/PyPDF3/blob/master/LICENSE
pyrsistent	http://github.com/tobgu/pyrsistent/	https://github.com/tobgu/pyrsistent/blob/master/LICENSE.mit
pysam	https://github.com/pysam-developers/pysam	https://github.com/pysam-developers/pysam/blob/master/COPYING
PySocks	https://github.com/Anorov/PySocks	https://github.com/Anorov/PySocks/blob/master/LICENSE
pytables	https://www.pytables.org	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
python	https://www.python.org/	https://docs.python.org/3/license.html
python-bidi	https://github.com/MeirKriheli/python-bidi	https://github.com/MeirKriheli/python-bidi/blob/master/COPYING
python-constraint	https://github.com/python-constraint/python-constraint	https://github.com/python-constraint/python-constraint/blob/master/LICENSE
python-dateutil	https://dateutil.readthedocs.io	https://github.com/dateutil/dateutil/blob/master/LICENSE
python-json-logger	http://github.com/madzak/python-json-logger	https://github.com/madzak/python-json-logger/blob/master/LICENSE

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Name of Project	Website	License URL
python-pptx	https://github.com/scanny/python-pptx	https://github.com/scanny/python-pptx/blob/master/LICENSE
python-ldap	https://www.python-ldap.org/	https://github.com/python-ldap/python-ldap/blob/python-ldap-3.4.0/LICENCE
python3-saml	https://github.com/onelogin/python3-saml	https://github.com/onelogin/python3-saml/blob/master/LICENSE
python_abi	https://github.com/conda-forge/python_abi-feedstock	https://github.com/conda-forge/python_abi-feedstock/blob/main/LICENSE.txt
pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning	https://github.com/Lightning-AI/pytorch-lightning/blob/master/LICENSE
pytz	https://pythonhosted.org/pytz	https://git.launchpad.net/pytz/tree/LICENSE.txt
pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim	https://github.com/pganssle/pytz-deprecation-shim/blob/master/LICENSE
PyWavelets	https://github.com/PyWavelets/pywt	https://github.com/PyWavelets/pywt/blob/master/LICENSE
PyYAML	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
pyyml	No longer available	No longer available
pyzmq	https://pyzmq.readthedocs.io/en/latest/	https://github.com/zeromq/pyzmq/blob/main/COPYING.BSD
qcelemental	https://github.com/MolSSI/QCElemental	https://github.com/MolSSI/QCElemental/blob/master/LICENSE

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Name of Project	Website	License URL
qcengine	https://github.com/MolSSI/QCEngine	https://github.com/MolSSI/QCEngine/blob/master/LICENSE
qrcode	https://github.com/lincolnloop/python-qrcode	https://github.com/lincolnloop/python-qrcode/blob/main/LICENSE
ramda	https://github.com/ramda/ramda	https://github.com/ramda/ramda/raw/master/LICENSE.txt
rapidjson	https://rapidjson.org/	https://github.com/Tencent/rapidjson/blob/master/license.txt
rdkit	https://www.rdkit.org	https://github.com/rdkit/rdkit/blob/master/license.txt
re2	https://github.com/google/re2	https://github.com/google/re2/blob/main/LICENSE
readme-renderer	https://github.com/pypa/readme_renderer	https://github.com/pypa/readme_renderer/blob/main/LICENSE
redis-py	https://github.com/andymccurdy/redis-py	https://github.com/redis/redis-py/blob/master/LICENSE
referencing	https://github.com/python-jsonschema/referencing	https://github.com/python-jsonschema/referencing
regex	https://github.com/mrabarnett/mrab-regex	https://github.com/mrabarnett/mrab-regex/blob/hg/LICENSE.txt
reportlab	https://www.reportlab.com	https://www.reportlab.com/dev/docs/faq/#1.3
reproc	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE
reproc-cpp	https://github.com/DaanDeMeyer/reproc	https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE

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Name of Project	Website	License URL
requests	https://requests.readthedocs.io	https://github.com/psf/requests/blob/main/LICENSE
requests-oauthlib	https://github.com/requests/requests-oauthlib	https://github.com/requests/requests-oauthlib/blob/master/LICENSE
requests-toolbelt	https://toolbelt.readthedocs.org	https://github.com/requests/toolbelt/blob/master/LICENSE
resumable	https://github.com/stevvooe/resumable	https://github.com/stevvooe/resumable/blob/master/LICENSE
retrying	https://github.com/rholder/retrying	https://github.com/rholder/retrying/blob/master/LICENSE
rfc3339-validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator/blob/master/LICENSE
rfc3339_validator	https://github.com/naimetti/rfc3339-validator	https://github.com/naimetti/rfc3339-validator?tab=MIT-1-ov-file#readme
rfc3986	https://rfc3986.readthedocs.io/en/latest/	https://github.com/python-hyper/rfc3986/blob/main/LICENSE
rfc3986-validator	https://github.com/naimetti/rfc3986-validator	https://github.com/naimetti/rfc3986-validator/blob/master/LICENSE
rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax	https://github.com/willynilly/rfc3987-syntax?tab=MIT-1-ov-file#readme
rich	https://github.com/Textualize/rich	https://github.com/Textualize/rich/blob/master/LICENSE

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Name of Project	Website	License URL
rich-argparse	https://github.com/hamdanal/rich-argparse	https://github.com/hamdanal/rich-argparse/blob/main/LICENSE
rlPyCairo	https://pypi.org/project/rlPyCairo/	https://hg.reportlab.com/hg-public/rlPyCairo/file/tip/rlPyCairo/LICENSE.txt
RocksDict	https://github.com/rocksdict/RocksDict	https://github.com/rocksdict/RocksDict?tab=MIT-1-ov-file#readme
roman-numerals	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
roman-numerals-py	https://github.com/AA-Turner/roman-numerals	https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme
rotary-embedding-torch	https://github.com/lucidrains/rotary-embedding-tor	https://github.com/lucidrains/rotary-embedding-tor blob/main/LICENSE
rpds-py	https://github.com/crate-py/rpds	https://github.com/crate-py/rpds
rpmpack	https://github.com/google/rpmpack	https://github.com/google/rpmpack/blob/master/LICENSE
rsa	https://stuvel.eu/rsa	https://github.com/sybrenstuvel/python-rsa/blob/main/LICENSE
ruamel-yaml	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/LICENSE
ruamel.yaml.clib	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/	https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/LICENSE

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Name of Project	Website	License URL
s3transfer	https://github.com/boto/s3transfer	https://github.com/boto/s3transfer/blob/develop/LICENSE.txt
sacrebleu	https://github.com/mjpost/sacrebleu	https://github.com/mjpost/sacrebleu/blob/master/LICENSE.txt
sapiens	https://github.com/Merck/Sapiens	https://github.com/Merck/Sapiens/blob/main/LICENSE
sasl	https://mellium.im/sasl	https://github.com/mellium/sasl/blob/main/LICENSE
scikit-gstat	https://mmaelicke.github.io/scikit-gstat/	https://github.com/mmaelicke/scikit-gstat/blob/main/LICENSE
scikit-image	https://scikit-image.org	https://scikit-image.org/docs/dev/license.html
scikit-learn	https://scikit-learn.org/stable/	https://github.com/scikit-learn/scikit-learn/blob/main/COPYING
scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra	https://github.com/scikit-learn-contrib/scikit-learn-extra/blob/main/LICENSE
scikit-network	https://github.com/sknetwork-team/scikit-network	https://github.com/sknetwork-team/scikit-network?tab=License-1-ov-file#readme
scipy	https://scipy.org	https://github.com/scipy/scipy/blob/main/LICENSE.txt
seaborn	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE
seaborn-base	https://seaborn.pydata.org	https://github.com/mwaskom/seaborn/blob/master/LICENSE

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Name of Project	Website	License URL
semver	https://github.com/Masterminds/semver/v3	https://github.com/Masterminds/semver/blob/v3.0.3/LICENSE.txt
Send2Trash	https://github.com/arsenetar/send2trash	https://github.com/arsenetar/send2trash/blob/master/LICENSE
sentry-sdk	https://github.com/getsentry/sentry-python	https://github.com/getsentry/sentry-python/blob/master/LICENSE
setproctitle	https://github.com/dvarrazzo/py-setproctitle	https://github.com/dvarrazzo/py-setproctitle/blob/master/LICENSE
setuptools	https://github.com/pypa/setuptools	https://github.com/pypa/setuptools/blob/main/LICENSE
setuptools-scm	https://github.com/pypa/setuptools_scm/	https://github.com/pypa/setuptools_scm/blob/main/LICENSE
sh	https://github.com/amoffat/sh	https://github.com/amoffat/sh/blob/develop/LICENSE.txt
shellingham	https://github.com/sarugaku/shellingham	https://github.com/sarugaku/shellingham/blob/master/LICENSE
simdjson	https://github.com/simdjson/simdjson/tree/master	https://github.com/simdjson/simdjson/blob/master/LICENSE
simint	https://www.bennyp.org/research/simint/	https://github.com/simint-chem/simint-generator/blob/master/LICENSE
simplejson	https://github.com/simplejson/simplejson	https://github.com/simplejson/simplejson/blob/master/LICENSE.txt
six	https://github.com/benjaminp/six	https://github.com/benjaminp/six/blob/master/LICENSE

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Name of Project	Website	License URL
smirnoff99frosst	https://github.com/openforcefield/smirnoff99frosst	https://github.com/openforcefield/smirnoff99Frosst/blob/master/LICENSE
smmap	https://github.com/gitpython-developers/smmap	https://github.com/gitpython-developers/smmap/blob/master/LICENSE
snappy	https://github.com/google/snappy	https://github.com/google/snappy/blob/main/COPYING
sniffio	https://github.com/python-trio/sniffio	https://github.com/python-trio/sniffio/blob/master/LICENSE.MIT
snowballstemmer	https://github.com/snowballstem/snowball	https://github.com/snowballstem/snowball/blob/master/COPYING
soupsieve	https://github.com/facelessuser/soupsieve	https://github.com/facelessuser/soupsieve/blob/main/LICENSE.md
spdlog	https://github.com/gabime/spdlog	https://github.com/gabime/spdlog?tab=License-1-ov-file#readme
spglib	https://spglib.readthedocs.io/	https://github.com/spglib/spglib/blob/develop/COPYING
sphinx	https://github.com/sphinx-doc/sphinx	https://github.com/sphinx-doc/sphinx/blob/5.x/LICENSE
sphinxcontrib-applehelp	https://github.com/sphinx-doc/sphinxcontrib-applehe	https://github.com/sphinx-doc/sphinxcontrib-applehe blob/master/LICENSE
sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp	https://github.com/sphinx-doc/sphinxcontrib-devhelp blob/master/LICENSE
sphinxcontrib-htmlhelp	https://github.com/sphinx-doc/sphinxcontrib-htmlhel	https://github.com/sphinx-doc/sphinxcontrib-htmlhel blob/master/LICENSE

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Name of Project	Website	License URL
sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath	https://github.com/sphinx-doc/sphinxcontrib-jsmath/blob/master/LICENSE
sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp	https://github.com/sphinx-doc/sphinxcontrib-qthelp/blob/master/LICENSE
sphinxcontrib-serializinghtml	https://github.com/sphinx-doc/sphinxcontrib-serializ	https://github.com/sphinx-doc/sphinxcontrib-serializ blob/master/LICENSE
SQLAlchemy	https://www.sqlalchemy.org	https://docs.sqlalchemy.org/en/14/copyright.html
SQLAlchemy	https://www.sqlalchemy.org/	https://github.com/sqlalchemy/sqlalchemy?tab=MIT-1-ov-file#readme
sqlite	https://sqlite.org/index.html	https://sqlite.org/copyright.html
sqlparse	https://github.com/andialbrecht/sqlparse	https://github.com/andialbrecht/sqlparse/blob/master/LICENSE
stack-data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data/blob/master/LICENSE.txt
stack_data	http://github.com/alexmojaki/stack_data	https://github.com/alexmojaki/stack_data?tab=MIT-1-ov-file#readme
starfile	https://github.com/alisterburt/starfile	https://github.com/teamtomo/starfile/blob/main/LICENSE
statsmodels	https://github.com/statsmodels/statsmodels	https://github.com/statsmodels/statsmodels/blob/main/LICENSE.txt
structlog	https://www.structlog.org/	https://github.com/hynek/structlog/blob/main/LICENSE

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Name of Project	Website	License URL
streamlit	https://github.com/streamlit/streamlit	https://github.com/streamlit/streamlit/blob/develop/LICENSE
svglib	https://github.com/deeplook/svglib	https://github.com/deeplook/svglib/blob/master/LICENSE.txt
sympy	https://sympy.org	https://github.com/sympy/sympy/blob/master/LICENSE
tables	https://www.pytables.org/	https://github.com/PyTables/PyTables/blob/master/LICENSE.txt
tabulate	https://github.com/astanin/python-tabulate	https://github.com/astanin/python-tabulate/blob/master/LICENSE
tbb	https://github.com/oneapi-src/oneTBB	https://github.com/oneapi-src/oneTBB/blob/master/LICENSE.txt
tenacity	https://github.com/jd/tenacity	https://github.com/jd/tenacity/blob/master/LICENSE
tensorboard	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-data-server	https://github.com/tensorflow/tensorboard	https://github.com/tensorflow/tensorboard/blob/master/LICENSE
tensorboard-plugin-wit	https://github.com/pair-code/what-if-tool	https://github.com/PAIR-code/what-if-tool/blob/master/LICENSE
tensorboardX	https://github.com/lanpa/tensorboardX	https://github.com/lanpa/tensorboardX/blob/master/LICENSE
tensorflow	https://github.com/tensorflow/tensorflow	https://github.com/tensorflow/tensorflow/blob/master/LICENSE

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Name of Project	Website	License URL
tensorflow-estimator	https://github.com/tensorflow/estimator	https://github.com/tensorflow/estimator/blob/master/LICENSE
tensorflow-io-gcs-filesystem	https://github.com/tensorflow/io	https://github.com/tensorflow/io/blob/master/LICENSE
tensorflow-probability	https://github.com/tensorflow/probability	https://github.com/tensorflow/probability/blob/main/LICENSE
termcolor	https://github.com/hugovk/termcolor	https://github.com/hugovk/termcolor/blob/main/COPYING.txt
terminado	https://github.com/jupyter/terminado	https://github.com/jupyter/terminado/blob/main/LICENSE
testpath	https://github.com/jupyter/testpath	https://github.com/jupyter/testpath/blob/master/LICENSE
textangular	https://github.com/fraywing/textAngular	https://github.com/fraywing/textAngular
texttable	https://github.com/foutaise/texttable/	https://github.com/foutaise/texttable/?tab=MIT-1-ov-file#readme
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
tf_keras	https://github.com/keras-team/keras-io	https://github.com/keras-team/keras-io/blob/master/LICENSE
threadpoolctl	https://github.com/joblib/threadpoolctl	https://github.com/joblib/threadpoolctl/blob/master/LICENSE
three	https://github.com/mrdoob/three.js	https://github.com/mrdoob/three.js/raw/master/LICENSE

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Name of Project	Website	License URL
tifffile	https://github.com/cgohlke/tifffile/	https://github.com/cgohlke/tifffile/blob/master/LICENSE
tinycss2	https://github.com/Kozea/tinycss2/	https://github.com/Kozea/tinycss2/blob/master/LICENSE
tinyxml2	https://github.com/leethomason/tinyxml2	https://github.com/leethomason/tinyxml2/blob/master/LICENSE.txt
tk	https://www.tcl.tk/	https://www.tcl.tk/software/tcltk/license.html
toml	https://github.com/toml-lang/toml	https://github.com/toml-lang/toml/blob/main/LICENSE
tomli	https://github.com/hukkin/tomli	https://github.com/hukkin/tomli/blob/master/LICENSE
toolz	https://github.com/pytoolz/toolz	https://github.com/pytoolz/toolz/blob/master/LICENSE.txt
torch	https://pytorch.org/	https://pypi.org/project/torch/#license
torch-geometric	https://pyg.org/	https://github.com/pyg-team/pytorch_geometric?tab=MIT-1-ov-file#readme
torcheval	https://github.com/pytorch/torcheval	https://github.com/pytorch/torcheval?tab=License-1-ov-file#readme
torchmetrics	https://github.com/Lightning-AI/torchmetrics	https://github.com/Lightning-AI/torchmetrics?tab=Apache-2.0-1-ov-file#readme
tornado	https://www.tornadoweb.org	https://github.com/tornadoweb/tornado/blob/master/LICENSE

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Name of Project	Website	License URL		
tqdm	https://github.com/tqdm/tqdm	https://github.com/tqdm/tqdm/blob/master/LICENCE		
tracy	https://github.com/gear-genomics/tracy	https://github.com/gear-genomics/tracy/blob/main/LICENSE		
traitlets	https://github.com/ipython/traitlets	https://github.com/ipython/traitlets/blob/main/COPYING.md		
triton	https://github.com/openai/triton/	https://github.com/openai/triton/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/trus	https://github.com/sethmlarson/truststore/blob/main/LICENSE		
truststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSEtruststore	https://github.com/sethmlarson/truststore	https://github.com/sethmlarson/truststore/blob/main/LICENSE
ts-jest	https://github.com/kulshekhar/ts-jest	https://github.com/kulshekhar/ts-jest/raw/master/LICENSE.md		
ts-loader	https://github.com/TypeStrong/ts-loader	https://github.com/TypeStrong/ts-loader/raw/master/LICENSE		
twine	https://github.com/pypa/twine	https://github.com/pypa/twine/blob/main/LICENSE		
twinj uuid	https://github.com/twinj/uuid	https://github.com/twinj/uuid/blob/master/LICENSE		
types	https://github.com/babel/babel	https://github.com/babel/babel/raw/master/LICENSE		
types-python-dateutil	https://github.com/python/typeshed	https://github.com/python/typeshed?tab=License-1-ov-file#readme		
types-requests	https://pypi.org/project/types-requests/	https://github.com/python/typeshed/blob/main/LICENSE		

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Name of Project	Website	License URL
typescript	https://github.com/Microsoft/TypeScript	https://github.com/Microsoft/TypeScript/raw/master/LICENSE.txt
typing-inspection	https://github.com/pydantic/typing-inspection	https://github.com/pydantic/typing-inspection?tab=MIT-1-ov-file#readme
typing-utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
typing_extensions	https://github.com/python/typing	https://github.com/python/typing/blob/master/LICENSE
typing_utils	https://github.com/bojiang/typing_utils	https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme
tzdata	https://github.com/python/tzdata	https://github.com/python/tzdata/blob/master/LICENSE
tzlocal	https://github.com/regebro/tzlocal	https://github.com/regebro/tzlocal/blob/master/LICENSE.txt
umf	https://github.com/oneapi-src/unified-memory-fram	https://github.com/oneapi-src/unified-memory-fram tab=License-1-ov-file#readme
umi-tools	https://github.com/CGATOxford/UMI-tools	https://github.com/CGATOxford/UMI-tools/blob/master/LICENSE
unicodedata2	https://github.com/fonttools/unicodedata2	https://github.com/fonttools/unicodedata2/blob/master/LICENSE
uri-template	https://gitlab.linss.com/open-source/python/uri-template	https://gitlab.linss.com/open-source/python/uri-template/-/blob/main/LICENSE
uritools	https://github.com/tkem/uritools/	https://github.com/tkem/uritools/blob/master/LICENSE

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Name of Project	Website	License URL		
urllib3	https://urllib3.readthedocs.io/	https://github.com/urllib3/urllib3/blob/main/LICENSE.txt		
vine	https://github.com/celery/vine	https://github.com/celery/vine/blob/master/LICENSE		
vue	https://github.com/vuejs/vue	https://github.com/vuejs/vue/raw/master/LICENSE		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readme		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readmewcwidth	https://github.com/jquast/wcwidth	https://github.com/jquast/wcwidth/blob/master/LICENSE
wandb	https://github.com/wandb/wandb	https://github.com/wandb/wandb/blob/main/LICENSE		
webcolors	https://github.com/ubernostrum/webcolors	https://github.com/ubernostrum/webcolors?tab=BSD-3-Clause-1-ov-file#readme		
webencodings	https://github.com/gsnedders/python-webencodings	https://github.com/gsnedders/python-webencodings/blob/master/LICENSE		
websocket-client	https://github.com/websocket-client/websocket-client.git	https://github.com/websocket-client/websocket-client/blob/master/LICENSE		
Werkzeug	https://palletsprojects.com/p/werkzeug/	https://werkzeug.palletsprojects.com/en/2.1.x/license/		
westpa	http://github.com/westpa/westpa	https://github.com/westpa/westpa/blob/westpa2/LICENSE		
wheel	https://github.com/pypa/wheel	https://github.com/pypa/wheel/blob/main/LICENSE.txt		

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Name of Project	Website	License URL
widgetsnbextension	https://github.com/jupyter-widgets/ipywidgets#readme	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE
wrapt	https://github.com/GrahamDumpleton/wrapt	https://github.com/GrahamDumpleton/wrapt/blob/develop/LICENSE
wsutil	https://github.com/yhat/wsutil	https://github.com/yhat/wsutil/blob/master/LICENSE
x/lint	https://golang.org/x/lint	https://github.com/golang/lint/blob/master/LICENSE
x/mod	https://golang.org/x/mod/semver	https://cs.opensource.google/go/x/mod/+/master:LICENSE
x/net	https://golang.org/x/net	https://cs.opensource.google/go/x/net/+/master:LICENSE
x/oauth2	https://golang.org/x/oauth2	https://cs.opensource.google/go/x/oauth2/+/master:LICENSE
x/sys	https://golang.org/x/sys	https://cs.opensource.google/go/x/sys/+/master:LICENSE
x/text	https://golang.org/x/text	https://cs.opensource.google/go/x/text/+/master:LICENSE
x/tools	https://golang.org/x/tools	https://cs.opensource.google/go/x/tools/+/master:LICENSE
x/xerrors	https://golang.org/x/xerrors	https://cs.opensource.google/go/x/xerrors/+/master:LICENSE
xgboost	https://github.com/dmlc/xgboost	https://github.com/dmlc/xgboost/blob/master/LICENSE
xhtml2pdf	http://github.com/xhtml2pdf/xhtml2pdf	https://github.com/xhtml2pdf/xhtml2pdf/blob/master/LICENSE.txt

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Name of Project	Website	License URL
xlrd	https://github.com/python-excel/xlrd	https://github.com/python-excel/xlrd/blob/master/LICENSE
xlsxwriter	https://github.com/jmcnamara/XlsxWriter	https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt
xmlsec	https://github.com/mehcode/python-xmlsec	https://github.com/mehcode/python-xmlsec/blob/master/LICENSE
xmltodict	https://github.com/martinblech/xmltodict	https://github.com/martinblech/xmltodict/blob/master/LICENSE
xorg-kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto/-/blob/master/COPYING
xorg-libice	https://gitlab.freedesktop.org/xorg/lib/libice	https://gitlab.freedesktop.org/xorg/lib/libice/-/blob/master/COPYING
xorg-libsm	https://gitlab.freedesktop.org/xorg/lib/libsm	https://gitlab.freedesktop.org/xorg/lib/libsm/-/blob/master/COPYING
xorg-libx11	https://gitlab.freedesktop.org/xorg/lib/libx11	https://gitlab.freedesktop.org/xorg/lib/libx11/-/blob/master/COPYING
xorg-libxau	https://gitlab.freedesktop.org/xorg/lib/libxau	https://gitlab.freedesktop.org/xorg/lib/libxau/-/blob/master/COPYING
xorg-libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp/-/blob/master/COPYING

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Table 1 – continued from previous page

Name of Project	Website	License URL
xorg-libxext	https://gitlab.freedesktop.org/xorg/lib/libxext	https://gitlab.freedesktop.org/xorg/lib/libxext/-/blob/master/COPYING
xorg-libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender/-/blob/master/COPYING
xorg-libxt	https://gitlab.freedesktop.org/xorg/lib/libxt	https://gitlab.freedesktop.org/xorg/lib/libxt/-/blob/master/COPYING
xorg-renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto/-/blob/master/COPYING
xorg-xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto/-/blob/master/COPYING
xorg-xproto	https://gitlab.freedesktop.org/xorg/proto/xproto	https://gitlab.freedesktop.org/xorg/proto/xproto/-/blob/master/COPYING
xxhash	https://github.com/cespare/xxhash/v2	https://github.com/cespare/xxhash/blob/main/LICENSE.txt
xz	https://github.com/ulikunitz/xz	https://github.com/ulikunitz/xz/blob/master/LICENSE
yaml	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
yaml-cpp	https://github.com/jbeder/yaml-cpp	https://github.com/jbeder/yaml-cpp/blob/master/LICENSE
yaml.v2	https://gopkg.in/yaml.v2	https://github.com/go-yaml/yaml/blob/v2.4.0/LICENSE
yaml.v3	https://gopkg.in/yaml.v3	https://github.com/go-yaml/yaml/blob/v3/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
yarl	https://github.com/aio-libs/yarl/	https://github.com/aio-libs/yarl/blob/master/LICENSE
yaspin	https://github.com/pavdmyt/yaspin	https://github.com/pavdmyt/yaspin/blob/master/LICENSE
yfiles	https://www.yworks.com/products/yfiles	commercial license
yml	https://pypi.org/project/yml/	N/A
zap	https://go.uber.org/zap	https://github.com/uber-go/zap/blob/master/LICENSE.txt
zipp	https://github.com/jaraco/zipp	https://github.com/jaraco/zipp/blob/main/LICENSE
zlib	https://zlib.net/	https://zlib.net/zlib_license.html
zstandard	https://github.com/indygreg/python-zstandard	https://github.com/indygreg/python-zstandard/blob/main/LICENSE
zstd	https://facebook.github.io/zstd/	https://github.com/facebook/zstd/blob/dev/LICENSE
click-option-group	https://github.com/click-contrib/click-option-group	https://github.com/click-contrib/click-option-group/blob/master/LICENSE

7.1 GCC

On the Linux platform, The OpenEye toolkits are linked with the GCC libraries using an eligible compilation process under the terms of the GCC RUNTIME LIBRARY EXCEPTION (see below).

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You should have received a copy of the GNU General Public License along with GCC (see below). If not, see Licenses GNU Project .

Per GPLv3, section 6d, the source for GCC is available for download from the following location: GNU. The GCC library components included here are from version gcc-4.9.3 and are built using the standard instructions at Installing GCC.

7.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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↪but changing it is not allowed.

This GCC Runtime Library Exception ("Exception") is an additional permission under␣
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of the file stating that the file is governed by GPLv3 along with this Exception.

When you use GCC to compile a program, GCC may combine portions of certain GCC header␣
↪files and runtime libraries with
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↪(including proprietary) programs
to use, in this way, the header files and runtime libraries covered by this Exception.

0. Definitions.

A file is an "Independent Module" if it either requires the Runtime Library for␣
↪execution after a Compilation Process,
or makes use of an interface provided by the Runtime Library, but is not otherwise based␣
↪on the Runtime Library.

"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
↪governed by version 3 (or a specified
later version) of the GNU General Public License (GPL) with the option of using any␣
↪subsequent versions published by the FSF.

"GPL-compatible Software" is software whose conditions of propagation, modification and␣
↪use would permit combination with
GCC in accord with the license of GCC.

"Target Code" refers to output from any compiler for a real or virtual target processor␣
↪architecture, in executable
form or suitable for input to an assembler, loader, linker and/or execution phase.␣
↪Notwithstanding that, Target Code
does not include data in any format that is used as a compiler intermediate␣
↪representation, or used for producing a
compiler intermediate representation.
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The "Compilation Process" transforms code entirely represented in non-intermediate␣
↪languages designed for human-written
code, and/or in Java Virtual Machine byte code, into Target Code. Thus, for example, use␣
↪of source code generators and
preprocessors need not be considered part of the Compilation Process, since the␣
↪Compilation Process can be understood
as starting with the output of the generators or preprocessors.

A Compilation Process is "Eligible" if it is done using GCC, alone or with other GPL-
↪compatible software, or if it is
done without using any work based on GCC. For example, using non-GPL-compatible Software␣
↪to optimize any GCC intermediate
representations would not qualify as an Eligible Compilation Process.

1. Grant of Additional Permission.

You have permission to propagate a work of Target Code formed by combining the Runtime␣
↪Library with Independent Modules,
even if such propagation would otherwise violate the terms of GPLv3, provided that all␣
↪Target Code was generated by
Eligible Compilation Processes. You may then convey such a combination under terms of␣
↪your choice, consistent with the
licensing of the Independent Modules.

2. No Weakening of GCC Copyleft.

The availability of this Exception does not imply any general presumption that third-
↪party software is unaffected by
the copyleft requirements of the license of GCC.
```

See also

- http://www.gnu.org/licenses/gcc-exception.html

7.1.2 GNU GENERAL PUBLIC LICENSE

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                    GNU GENERAL PUBLIC LICENSE
                       Version 3, 29 June 2007

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authors' sake, the GPL requires that modified versions be marked as
changed, so that their problems will not be attributed erroneously to
authors of previous versions.

  Some devices are designed to deny users access to install or run
modified versions of the software inside them, although the manufacturer
can do so.  This is fundamentally incompatible with the aim of
protecting users' freedom to change the software.  The systematic
pattern of such abuse occurs in the area of products for individuals to
use, which is precisely where it is most unacceptable.  Therefore, we
have designed this version of the GPL to prohibit the practice for those
products.  If such problems arise substantially in other domains, we
stand ready to extend this provision to those domains in future versions
of the GPL, as needed to protect the freedom of users.

  Finally, every program is threatened constantly by software patents.
States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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patents cannot be used to render the program non-free.

  The precise terms and conditions for copying, distribution and
modification follow.

                    TERMS AND CONDITIONS

  0. Definitions.

  "This License" refers to version 3 of the GNU General Public License.

  "Copyright" also means copyright-like laws that apply to other kinds of
works, such as semiconductor masks.

  "The Program" refers to any copyrightable work licensed under this
License.  Each licensee is addressed as "you".  "Licensees" and
"recipients" may be individuals or organizations.

  To "modify" a work means to copy from or adapt all or part of the work
in a fashion requiring copyright permission, other than the making of an
exact copy.  The resulting work is called a "modified version" of the
earlier work or a work "based on" the earlier work.

  A "covered work" means either the unmodified Program or a work based
on the Program.

  To "propagate" a work means to do anything with it that, without
permission, would make you directly or secondarily liable for
infringement under applicable copyright law, except executing it on a
computer or modifying a private copy.  Propagation includes copying,
distribution (with or without modification), making available to the
public, and in some countries other activities as well.

  To "convey" a work means any kind of propagation that enables other
parties to make or receive copies.  Mere interaction with a user through
a computer network, with no transfer of a copy, is not conveying.

  An interactive user interface displays "Appropriate Legal Notices"
to the extent that it includes a convenient and prominently visible
feature that (1) displays an appropriate copyright notice, and (2)
tells the user that there is no warranty for the work (except to the
extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

  The "source code" for a work means the preferred form of the work
for making modifications to it.  "Object code" means any non-source
form of a work.
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  A "Standard Interface" means an interface that either is an official
standard defined by a recognized standards body, or, in the case of
interfaces specified for a particular programming language, one that
is widely used among developers working in that language.

  The "System Libraries" of an executable work include anything, other
than the work as a whole, that (a) is included in the normal form of
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Component, and (b) serves only to enable use of the work with that
Major Component, or to implement a Standard Interface for which an
implementation is available to the public in source code form.  A
"Major Component", in this context, means a major essential component
(kernel, window system, and so on) of the specific operating system
(if any) on which the executable work runs, or a compiler used to
produce the work, or an object code interpreter used to run it.

  The "Corresponding Source" for a work in object code form means all
the source code needed to generate, install, and (for an executable
work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
System Libraries, or general-purpose tools or generally available free
programs which are used unmodified in performing those activities but
which are not part of the work.  For example, Corresponding Source
includes interface definition files associated with source files for
the work, and the source code for shared libraries and dynamically
linked subprograms that the work is specifically designed to require,
such as by intimate data communication or control flow between those
subprograms and other parts of the work.

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  You may convey a work based on the Program, or the modifications to
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terms of section 4, provided that you also meet all of these conditions:

   a) The work must carry prominent notices stating that you modified
   it, and giving a relevant date.

   b) The work must carry prominent notices stating that it is
   released under this License and any conditions added under section
   7.  This requirement modifies the requirement in section 4 to
   "keep intact all notices".
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    c) You must license the entire work, as a whole, under this
    License to anyone who comes into possession of a copy.  This
    License will therefore apply, along with any applicable section 7
    additional terms, to the whole of the work, and all its parts,
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    permission to license the work in any other way, but it does not
    invalidate such permission if you have separately received it.

    d) If the work has interactive user interfaces, each must display
    Appropriate Legal Notices; however, if the Program has interactive
    interfaces that do not display Appropriate Legal Notices, your
    work need not make them do so.

  A compilation of a covered work with other separate and independent
works, which are not by their nature extensions of the covered work,
and which are not combined with it such as to form a larger program,
in or on a volume of a storage or distribution medium, is called an
"aggregate" if the compilation and its resulting copyright are not
used to limit the access or legal rights of the compilation's users
beyond what the individual works permit.  Inclusion of a covered work
in an aggregate does not cause this License to apply to the other
parts of the aggregate.

  6. Conveying Non-Source Forms.

  You may convey a covered work in object code form under the terms
of sections 4 and 5, provided that you also convey the
machine-readable Corresponding Source under the terms of this License,
in one of these ways:

  a) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by the
  Corresponding Source fixed on a durable physical medium
  customarily used for software interchange.

  b) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by a
  written offer, valid for at least three years and valid for as
  long as you offer spare parts or customer support for that product
  model, to give anyone who possesses the object code either (1) a
  copy of the Corresponding Source for all the software in the
  product that is covered by this License, on a durable physical
  medium customarily used for software interchange, for a price no
  more than your reasonable cost of physically performing this
  conveying of source, or (2) access to copy the
  Corresponding Source from a network server at no charge.

  c) Convey individual copies of the object code with a copy of the
  written offer to provide the Corresponding Source.  This
  alternative is allowed only occasionally and noncommercially, and
  only if you received the object code with such an offer, in accord
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   with subsection 6b.

   d) Convey the object code by offering access from a designated
   place (gratis or for a charge), and offer equivalent access to the
   Corresponding Source in the same way through the same place at no
   further charge.  You need not require recipients to copy the
   Corresponding Source along with the object code.  If the place to
   copy the object code is a network server, the Corresponding Source
   may be on a different server (operated by you or a third party)
   that supports equivalent copying facilities, provided you maintain
   clear directions next to the object code saying where to find the
   Corresponding Source.  Regardless of what server hosts the
   Corresponding Source, you remain obligated to ensure that it is
   available for as long as needed to satisfy these requirements.

   e) Convey the object code using peer-to-peer transmission, provided
   you inform other peers where the object code and Corresponding
   Source of the work are being offered to the general public at no
   charge under subsection 6d.

  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
included in conveying the object code work.

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
or household purposes, or (2) anything designed or sold for incorporation
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doubtful cases shall be resolved in favor of coverage.  For a particular
product received by a particular user, "normally used" refers to a
typical or common use of that class of product, regardless of the status
of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
commercial, industrial or non-consumer uses, unless such uses represent
the only significant mode of use of the product.

  "Installation Information" for a User Product means any methods,
procedures, authorization keys, or other information required to install
and execute modified versions of a covered work in that User Product from
a modified version of its Corresponding Source.  The information must
suffice to ensure that the continued functioning of the modified object
code is in no case prevented or interfered with solely because
modification has been made.

  If you convey an object code work under this section in, or with, or
specifically for use in, a User Product, and the conveying occurs as
part of a transaction in which the right of possession and use of the
User Product is transferred to the recipient in perpetuity or for a
fixed term (regardless of how the transaction is characterized), the
Corresponding Source conveyed under this section must be accompanied
by the Installation Information.  But this requirement does not apply
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if neither you nor any third party retains the ability to install
modified object code on the User Product (for example, the work has
been installed in ROM).

  The requirement to provide Installation Information does not include a
requirement to continue to provide support service, warranty, or updates
for a work that has been modified or installed by the recipient, or for
the User Product in which it has been modified or installed.  Access to a
network may be denied when the modification itself materially and
adversely affects the operation of the network or violates the rules and
protocols for communication across the network.

  Corresponding Source conveyed, and Installation Information provided,
in accord with this section must be in a format that is publicly
documented (and with an implementation available to the public in
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