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Modeling Macro-Molecular Interfaces with `Intervor`

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Abstract: `Intervor` is a software computing a parameter free representation of macro-molecular interfaces, based on the α-complex of the atoms. Given two interacting partners, possibly with water molecules squeezed in-between them, `Intervor` computes an interface model which has the following characteristics: (i) it identifies the atoms of the partners which are in direct contact and those whose interaction is water mediated, (ii) it defines a geometric complex separating the partners, the Voronoi interface, whose geometric and topological descriptions are straightforward (surface area, number of patches, curvature), (iii) it allows the definition of the depth of atoms at the interface, thus going beyond the traditional dissection of an interface into a core and a rim.

These features can be used to investigate correlations between structural parameters and key properties such as the conservation of residues, their polarity, the water dynamics at the interface, mutagenesis data, etc.

`Intervor` can be run from the web site `http://cgal.inria.fr/abs/Intervor`, or in stand-alone mode upon downloading the binary file. Plugins are also made available for Visual Molecular Dynamics (VMD) and Pymol.

Key-words: Union of balls, Voronoi diagrams, α-shapes, proteins, macro-molecular complexes, interfaces, structural biology.

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Modélisation d'Interfaces Macro-Moléculaires avec `Intervor`

Résumé : `Intervor` est un logiciel calculant une représentation des interfaces macro-moléculaires basée sur l'α-complexe des atomes. Étant donnés deux partenaires, entre lesquels peuvent se trouver des molécules d'eau, l'interface calculée a les caractéristiques suivantes: (i) elle identifie les atomes en contact direct, ainsi que ceux dont l'interaction est écrantée par des molécules d'eau, (ii) elle définit un complexe cellulaire, l'interface de Voronoï, qui sépare les partenaires, et dont les caractéristiques géométriques et topologiques peuvent être aisément calculées, et (iii) elle permet le calcul de la profondeur des atomes à l'interface, permettant ainsi d'aller au-delà du modèle classique de zone centrale et de zone périphérique.

Ces paramètres peuvent être utilisés pour étudier les corrélations avec des quantités biophysiques importantes telles que la conservation des résidus, leur polarité, la dynamique du solvant à l'interface, des données de mutagénèse, etc.

`Intervor` peut être exécuté à partir du site web `http://cgal.inria.fr/abs/Intervor`, ou en ligne de commande avec le binaire disponible sur ce site. Des plugins sont disponibles pour Visual Molecular Dynamics (VMD) et Pymol.

Mots-clés : Union de boules, diagrammes de Voronoi, α-shapes, protéines, complexes macro-moléculaires, interfaces, biologie structurale.

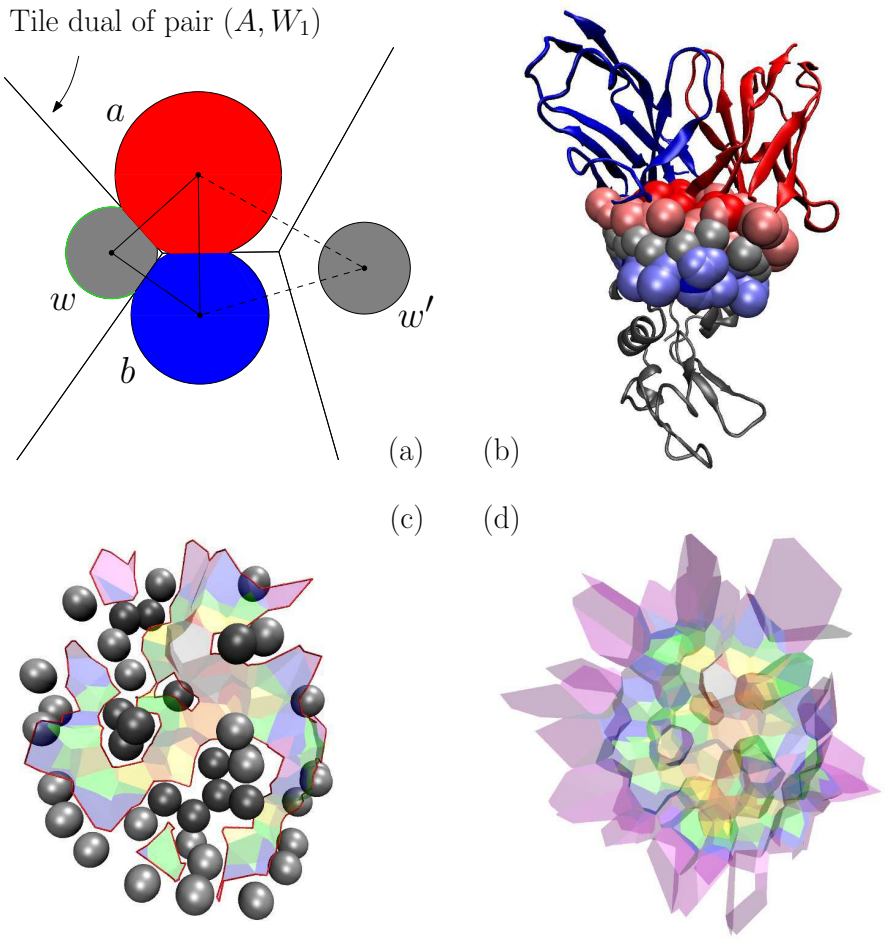

Figure 1: (a) A complex with two atoms (red and blue) and two water molecules (in grey). The interface comprises three pairs namely $[a; b]$, $[a; w]$, and $[b; w]$; water w' is not at the interface. (b) Antibody-antigen complex (1vfb.pdb) : chains and interface atoms displayed with radii expanded by 1.4$\mathring{A}$, with interface water molecules in grey. (c) 1vfb: Rotated view of the AB interface (colored tiles), and water molecules squeezed in-between partners. (d) 1vfb: Transparent view of the Voronoi shelling of the ABW interface into concentric shells. See text for details.

1 Introduction

Protein - protein recognition plays a key role in the formation of complexes which account for biological functions [9]. The investigation of interfaces of macro-molecular complexes is therefore central to improve our understanding of the stability and specificity of macro-molecular interactions. In conducting such investigations, one wishes to (i) improve the description of experimentally resolved complexes, and (ii) improve scoring functions used to discriminate native structures amongst putative ones. The goal of this note is to present an integrated interface model refining most of the parameters used so far in interface studies, using a unique parameter-free geometric construction.

2 The Voronoi interface

In the following, we consider two partners A and B forming a complex. By W, we refer to interfacial water molecules, if any. Abusing terminology, an atom of type A belongs to partner A, and similarly for B and W.

Traditional interface models. Two interface models are traditionally used: the geometric footprint based model, which consists in considering all pairs of atoms (one on each partner) within some distance threshold;

the solvent accessible model, which selects atoms losing solvent accessibility upon complex formation. While the former tends to overestimate the interface size [7], the opposite holds for the latter [3]. This motivates our Voronoi interface model.

The Voronoi interface model: direct versus water mediated contacts. Consider the power diagram of the atomic balls expanded by a water probe—abusing terminology we call it the Voronoi diagram in the sequel. Let a *restricted ball* or *restriction* be the intersection of this ball with its Voronoi region, see e.g. the red ball on Fig. 1(a). Also, let an *interface water molecule* be a water molecule such that its restriction has neighboring restrictions of type A and B. Water molecules which are not at the interface are called *bulk* water molecules. Our interface model consists of pairs of restrictions of type $[A;B]$ or $[A;W]$ or $[B;W]$, with W standing for interface water molecule only. See Fig. 1(a). Note that every such pair conveys two pieces of information: (i) the two atoms in contact, which define an interface edge, and (ii) the Voronoi facet, also called *tile*, dual of this edge.

All atoms involved in at least one pair define the interface atoms, as illustrated on Fig. 1(b). A tile of type AB defines a direct contact between atoms of the partners, while interface water molecules mediate interactions between these partners. We define the interface AB (respectively $AW-BW$) as the collection of tiles of type AB (respectively AW or BW). See Fig. 1(c). Also, we define the interface ABW as the union of the AB and $AW-BW$ interfaces. The ABW interface separates the partners and gives a global overview of the interaction area, regardless of the particular role played by water molecules.

Shelling the Voronoi interface. Think of a room whose floor is tiled, the room being delimited by walls. Assign the integer one to all tiles in contact with a wall. Having removed these tagged tiles, move the walls towards the tiles which were in contact with them, and tag these with the integer two. Iterating the process until completion results in a discrete numbering measuring the minimum distance from a tile to the boundary of the room. This process is carried out for the tiles of the ABW interface, starting from its boundary, the resulting number being called the *Voronoi Shelling Order* or *VSO*. See Fig. 1(d). Since an interface atom contributes at least one tile, the VSO of this atom is defined as the minimum of the values found on the tiles contributed by this atom.

Connexions to classical interface parameters. We established that our model identifies a superset of interface atoms losing solvent accessibility [1], which actually draws the attention to interactions between main chain atoms upon association [3]. Interface tiles are naturally gathered into patches, which have been shown [3] to be coherent with those obtained with classical clustering algorithms [4]. Quantifying the planarity of interfaces and patches is important, e.g. to estimate (de-)solvation energies and also to identify putative binding regions for docking. While previous studies have used strategies based on plane fitting [10], the Voronoi interface comes with a notion of discrete (mean) curvature, which allows to assess the curvature properties at any scale (from two tiles to the whole interface).

Finally, the VSO provides a discrete interface depth parameterization which refines the dissection into a core and a rim [5, 1]. This parameterization allowed us to sharpen the investigation of correlations between (i) the interface geometry, (ii) the location of polar residues [4], (iii) the location of conserved residues [8], (iv) the dynamics of interfacial water [11].

3 Using `Intervor`

Availability. `Intervor` is made available from `http://cgal.inria.fr/abs/Intervor/`. This web site allows one (i) to run calculations, and (ii) to retrieve the binary file. In presenting the software, we briefly discuss the main options, and refer the user either to the web site or the help provided from the command line with the `--help` option. See also [3, 2] to get familiar with the structural parameters computed.

Atomic and coarse models. `Intervor` is written is C++, and our code handles balls, be they atoms or pseudo-atoms. Because of the diversity of radii sets used for pseudo-atoms, we focus in the sequel on the atomic version.

Specifying the system. First, one needs to select which atoms define the two partners A and B. The standard way consists of selecting chains within a PDB file. Second, one needs to sort out the fate of water molecules if any: one can keep them all, skip them all, or filter them on their temperature factor. Once the water molecules have been filtered, they are incorporated into the Voronoi diagram, and the interface water molecules are identified. See Fig. 1(a).

Running `Intervor` and output files. To understand the structure of the output, any `Intervor` execution goes through four steps, namely (i) interface water molecules are identified (ii) interface AB is explored (iii)

interface $AW - BW$ is explored (iv) interfaces AB and $AW - BW$ are merged. The output consists of six files. The main log file provides general information; the remaining ones provide detailed statistics on interface atoms and the Voronoi interface. See the supplemental for the details.

Visualization. Plugins are made available to run a calculation on a structure and to load the result within VMD or Pymol. Visualization facilities target atoms and the Voronoi interface. For the former, atoms of each partner and water molecules can be visualized independently. Each set of atoms of type A or B or W is presented in two guises, namely with Van der Waals or expanded radii. Interfaces AB and $AW - BW$ interfaces can be visualized independently.

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4 Files generated by `Intervor`

In the following, we describe the files generated by `Intervor`, and refer the reader to [6] for a description of the geometry underlying the interface construction, and to [3, 2] for applications to structural studies.

4.1 Conventions

`Intervor` generates files containing pieces of information about interface atoms and their contacts. When dumping a given atom, we use the plain PDB format, or the *reduced PDB format*, which consists of the following four-tuple: atom serial number, PDB atom name, residue name and chain id.

All atoms of a PDB file are assigned to five types: A and B for the two partners, W_b and W_i for the bulk and interface water molecules, and X for the remaining atoms. (As mentioned in section 3, recall that the water molecules loaded into the Voronoi diagram are classified either as interfacial or bulk.) In the files generated by `Intervor`, these types are respectively denoted `IA_A`, `IA_B`, `IA_Wb`, `IA_Wi`, `IA_X`. (Prefix `IA` stands for Interface Atom.)

The five atomic types are used to define types for pairs, in particular types AB, AW_i and BW_i which are used to define the AB and $AW-BW$ interfaces. In the output files, these types are denoted `IE_AB`, `IE_AWi` and `IE_BWi`. (Prefix `IE` stands for Interface Edge.)

These five types are also used to define so-called manifold interfaces: a manifold interface is a subset of the Voronoi diagram such that any Voronoi edge is incident to at most two Voronoi faces. Of particular interest are the following manifold interfaces, also called bicolor interfaces: AB, AW_i, BW_i. The collection of all tiles of type AW_i and BW_i define the $AW-BW$ interface. In the output files, these interfaces are respectively denoted `MI_AB`, `MI_AWi`, `BWi`, `MI_AWi_BWi`. (Prefix `MI` stands for Manifold Interface.) We note in passing that the ABW interface is not a manifold one, since three Voronoi facets can be incident on the same Voronoi edge.

From a biochemical standpoint, we use an annotation with 15 entries. See the web site for details [1]. To investigate pairwise interactions, any pair of atoms within the $15\times16/2$ pairs of chemical annotations is assigned a type with a set of size 10.

4.2 Overview of files generated

When called on a file `fprefix.pdb`, `Intervor` generates six files. These files are self-contained, whence some redundancy, and provide a description of the two complementary aspects of interface modeling: interface atoms and Voronoi interface. These files, which are described in section 4.3, are the following ones:

`fprefix_log-IV.txt`**: general.** This file is only generated when `Intervor` is called with the `--log` option; otherwise, its content is dumped onto the standard output. Information provided is high-level information: number of interface patches and corresponding statistics, number of atoms, number of pairs, etc. The remaining files detail this information.

`fprefix_iar-IV.txt`**: interface atoms.** The list of interface atoms in text format, together with selected annotations.

`fprefix_iar-IV.pdb`**: interface atoms.** The list of interface atoms in PDB format. The atom serial number reported is that of the original file.

`fprefix_contacts-IV.txt`**: pairs of atoms.** The pairwise contacts.

`fprefix_interface-IV.txt`**: Voronoi interface.** Geometric and topological description of the Voronoi interface.

`fprefix_patches-IV.txt`**: patches of the Voronoi interface.** Dissection of the interface atoms as a function of the patches they participate to.

[1] Note that type and annotation respectively refer to the classifications with 5 and 15 types.

4.3 Description of files generated

To describe a given file, we provide a textual description accompanied by a copy-paste of the output on the antibody - antigen complex 1vfb, which contains interfacial water. In the copy-paste section, the macro `MUTATIS MUTANDIS` is used to indicate that part of the output has the structure of an already discussed piece of output. Also, `ETC` means that the copy-pasted region has been shortened.

4.3.1 File `fprefix_log-IV.txt`

Information provided in this file splits into three sections. The first two are present in any case; the third one is found if and only if interface water molecules are detected.

▷ **Description: File header.**

The header lists general statistics about the complex:
– number of (finite) simplices of each dimension in the Delaunay triangulation underlying the construction (vertices, edges, triangles, tetrahedra).
– the types of atoms used, and the corresponding radii.
– the number of water molecules found at the interface.
– the number of atoms and the number of interface atoms, classified into the five aforementioned types, namely A, B, W_b, W_i, X, together with the number of interface atoms classified in the 15 aforementioned chemical annotations.
– for the three types of interface edges AB, AW_i and BW_i, the number of such edges, the number of edges discarded if filtering on the Voronoi facet size is active [2], and the number of edges found on the convex hull. (Note that such edges are automatically discarded if filtering by size is active.)
– the number of Voronoi facets processed while computing the Voronoi shelling order.

▷ **Verbatim.**

```
+-+Partners_classifier::dump_specs:
 0; chain(s): <AB>
 1; chain(s): <C>
+-+AppliManager_flow::load_fileTriangul infos: #simplices [Vces -> Tetras]: 2779 21162 36685 18301

+-+Partners: #atoms kept  [A B Wb X]: 1730 1001 48 0
+-+Chemical annotations
+-+Radius used for Cali 1.87
+-+Radius used for Caro 1.76
ETC

+++AS_interf_toolbox::tag_interf_atoms_classify_edges...
+-+Re-labelling Wb to Wi: 39
+-+Atoms_residues::#atoms [A B Wb Wi X]: 1730 1001 9 39 0
+-+Atoms_residues::#iatoms [A B Wb Wi X]: 155 135 0 39 0
+-+Atoms_residues::#interf atoms annotated: Cali: 88 Caro: 67 Cpep: 25 Nhbd: 34 Naro: 4 ETC

+-+Filtering edges on Voronoi facet size: no
+-+Edges of type IE_A_B: #OK #TooLarge #ConvexHull : 240 0 0
+-+Edges of type IE_A_Wi: #OK #TooLarge #ConvexHull : 263 0 0
+-+Edges of type IE_B_Wi: #OK #TooLarge #ConvexHull : 248 0 0
+-+Total #edges 751
+++AS_interf_toolbox::tag_interf_atoms_classify_edges

+++VSO_shelling_from_boundary...
+-+Interf_explorer_SO::starting with 132 boundary vor edges
+-+Interf_explorer_SO::shelled 751 vor facets
---VSO_shelling_from_boundary
```

▷ **Description: Interface AB.**

Information on interface AB splits into three sections.

First, each connected component (cc) is described. These cc, which are indexed in-between 0 and $n-1$ if there are n of them, are described by:

[2] Recall that a Voronoi facet is considered too large iff the ratio between the squared radii of the largest orthogonal ball to the two balls dual of the facet and the minimum squared radii of these two balls is beyond a user-defined threshold. This filtering mechanism in only meant to avoid excessively large facets in the VMD or Pymol display engine. See [6, 3] for the details.

–the type of edge the cc was started with, the number of Voronoi facets and their surface area in $\mathring{A}^2$, followed by the number of {boundary loops, internal edges, boundary edges}.
–the atomic composition i.e. the number of atoms of the five types.
–the number of edges of each boundary loop bounding the cc.

Second, three lines summarize interface properties:
–a summary of global statistics for all connected components of the interface: number of { cc, faces, boundary edges, loops}.
–the surface area information, in $\mathring{A}^2$, dissected in terms of pairs (of atoms types and of chemical annotations).

Third, we get the curvature information $sAbsH$ and sH—see [3], together with the surface area of Voronoi facets, denoted sA, and the length of the boundary loops, denoted sL. The last two lines provide the average and standard deviation of the dihedral angle $\beta(e)$ between incident Voronoi facets, and its absolute value, in radians.

▷ **Verbatim.**

```
+-+Exploring interface MI_AB
 0 IE_A_B; #facets:  226 area:  440.30  #loops:   2 #int_edges: 456
#bd_edges: 196; Atom comp. [78;62;0;0;0];\
 loop lengths [181 15]

MUTATIS MUTANDIS for the other connected components

+-+MI::dump_interf_stats:: #ccs / #facets / #bd_edges / #loops: 3 240 230 4
+-+Surf_areas::Interface areas<MI_AB>: IE_A_B: 467.58
+-+Surf_areas::Chem Interface areas<MI_AB>: ali: 186.47 aro: 17.22 hbd: 80.19 hbw: 0.00 hbdp: 0.00\
 elu: 0.00 elf: 0.00 hbwp: 0.00 ssb: 0.00 unk: 183.70

+-+MI::mean curvature-a sH sAbsH:          -63.53 583.69
+-+MI::mean curvature-b sA sL:             467.58 1016.32
+-+MI::mean curvature-c sH/sA sAbsH/sA:    -0.14 1.25
+-+MI::signed   angle mu sigma: -0.06 0.65
+-+MI::signless angle mu sigma: 0.57 0.31
```

▷ **Description: Interfaces $AW-BW$ and ABW.**

If water molecules have been found at the interface, we first report for the $AW-BW$ interface all the information just outlined for the AB interface.

Next, we detail the Union-Find process which builds the interface ABW by merging the interfaces AB and $AW-BW$. Recall that this information tells us to which extent water molecules merge gaps in-between the patches corresponding to direct interactions between the partners.

The elementary merge operation consists of merging two connected components along a common Voronoi edge. This edge may belong to two boundary loops of two connected components of the AB and $AW-BW$ interfaces, or may involve one boundary and one interior Voronoi edge. Statistics are reported for each connected component of the merge. First, one finds information on the Union-Find process itself, namely the number of interior and boundary Voronoi edges involved in the process, together with the number of components and loops after the merge. Second, each component is detailed. We indicate for each boundary net the number of loops involved. Finally, we provide the facet area information for the merged connected components, dissected in terms of pairs (of atoms types and of chemical annotations).

▷ **Verbatim.**

```
+-+Exploring interface MI_AWi_BWi

MUTATIS MUTANTIS wrt interface MI_AB

+-+UnionFindAlgo::union_find
 #CCS FromTo: 10 1
 #loops FromTo: 18 15

+++UnionFindAlgo::process_merged_ccs #0
Start boundary net with  1 loops
ETC

+-+Surf_areas::Interface areas<for merged connected component>: A_B: 467.58 A_Wi: 454.93 B_Wi: 455.13
+-+Surf_areas::Chem Interface areas<for merged connected component>: ali: 186.47 aro: 17.22 hbd: 80.19 hbw: 438.06\
```

```
 hbdp: 0.00 elu: 0.00 elf: 0.00 hbwp: 0.00 ssb: 0.00 unk: 655.70
+-+MCC_record::dump_stats::Nb loops_before - nets_after uf merge: 18 15
---UnionFindAlgo::process_merged_ccs #0 done

MUTATIS MUTANDIS for the remaining merged cc, if any
```

4.3.2 File `fprefix_iar-IV.txt`

▷ Description: Connectivity of atoms.

This file splits into two parts.

The first one collects information about interface atoms. For each of the three types A, B, W_i, one gets one line per atom, with the following information:
– First, the reduced PDB entry is provided.
– Second, the type is recalled, together with a boolean stating whether the atoms is buried (true) or exposed (false), and the chemical annotation.
– Third, one finds 3 integers: the minimum and maximum of the Voronoi Shelling Order (VSO), followed by -1 (placeholder to accommodate alternative definitions of depth). (Recall that the VSO is defined on a per Voronoi facet basis: since an atom can contribute several facets, its has a range of VSO instead of a single value.)
– Finally, the number of neighbors of the five types is provided.

Upon listing all interface atoms of that type, one finds a summary of the connectivity for this group of atoms, that is, the number of edges connecting atoms of this type to atoms of the 5 types.

The second part of the file contains information about bicolor interfaces $XY \in \{AB, AW, BW_i, W_iW_i\}$. For a given type, one finds a summary of connectivity information: the average number of neighbors of the second type, the numbers of atoms of both types, the number of edges of the bicolor interface.

▷ Verbatim.

```
Atoms of type IA_A
  236  ND2 ASN A  28; IA_A 0       Nhbd; 1 1 -1; 9 0 1 1 0
ETC

Buried/exposed summary for atom type IA_A [tot=155]: 97 58
Connectivity to five types ie nb edges: 1681 240 30 263 0

MUTATIS MUTANDIS for type IA_B

MUTATIS MUTANDIS for type IA_Wi

+-+Atoms_residues::dump_ave_interface_connectivity...
Average connectivity for edges of type IE_A_B
Atom type - neighbors type IA_A IA_B : 2.93
Atom type - neighbors type IA_B IA_A : 3.33
#IA_A: 82   #IA_B: 72   #e: 240

MUTATIS MUTANDIS for edges of type IE_A_Wi

MUTATIS MUTANDIS for edges of type IE_B_Wi
```

4.3.3 File `fprefix_iar-IV.pdb`

▷ Description: Interface atoms in PDB format.

A subset of the PDB file processed: one line for each interface atom.

▷ Verbatim.

```
ATOM    236 ND2  ASN A  28      34.584   1.642   8.811  1.00 23.36
ATOM    235 OD1  ASN A  28      35.268   2.367   6.845  1.00 19.73
ETC
```

4.3.4 File `fprefix_contacts-IV.txt`

▷ **Description: Pairwise contacts.**

For each XY interface, with X and Y atom types $\in \{A, B, W_i\}$, assuming $X < Y$ according to the lexicographic order, we dump interface pairs in reduced PDB format, together with the chemical annotation of the interaction.

▷ **Verbatim.**

```
IE_A_B pairs:
  876  CZ3 TRP A  92 3361   CD ARG C 125 ali
  877  CH2 TRP A  92 3361   CD ARG C 125 ali
ETC

MUTATIS MUTANDIS for pairs of type IE_A_Wi

MUTATIS MUTANDIS for pairs of type IE_B_Wi

MUTATIS MUTANDIS for pairs of type IE_Wi_Wi
```

4.3.5 File `fprefix_interface-IV.txt`

▷ **Description: The Voronoi interface.**

The Voronoi interface consists of Voronoi facets, each being the dual of an interface edge, and is bounded by loops and nets respectively before and after the merge of the AB and $AW - BW$ interfaces.

Before the merge process. For the manifold interfaces AB and $AW - BW$, the following pieces of information are dumped.

Voronoi Shelling Order. For each interface edge, represented by the atom serial numbers, one finds the value of VSO.

Voronoi facet. For each interface Voronoi facet, the following pieces of information are provided within the tags `FBeg` and `FEnd`. First encounters the two atoms involved, in reduced PDB format, together with the annotation of the interaction. Second, one finds the xyz coordinates of the atoms. Finally, the list of coordinates of the Voronoi centers bounding the facet is provided.

Boundary loops of a connected component. Once all the facets of the interface have been dumped, we get for each connected component the description of the boundary loops. Each loop is described as follows:
–the loop id (an integer between 1 and the total number of loops created for all interfaces), and the bicolor edge associated to the creation of the connected component this loop belongs to;
–a list of Voronoi vertices bounding the loop;
–two positive real numbers giving the sum of the total length of the loop, and the sum of the lengths of boundary edges. Before the merge process, all edges of a loop are boundary edges, so that the two values agree.

Facet Surface areas. Two dissections of the Voronoi Interface Area are provided: in terms of pairs (of atoms types and of chemical annotations).

After the merge process. After the merge process, we reconsider for each connected component the structure of loops and nets, and the dissection of the surface area of the merged components.

Boundary nets after Union-Find. During the merge process, all edges common to two components get identified, so that the length of the boundary edges of the net is less than its total length. These two values are reported. (Notice that a merge occurs in two situations: the two edges are boundary edges; or a boundary edge merges with an edge in the interior of a component.)

Voronoi Interface Area. The two dissections mentioned before the merge process are also reported.

▷ **Verbatim.**

```
Begin VSO per interface edge
236 3439  1
ETC

Voronoi Facets of interface MI_AB
FBeg
```

```
  876  CZ3 TRP A  92  3361   CD ARG C 125 ali
36.604 -4.459 4.408 33.831 -7.962 3.218  0.28
34.975952 -5.796048 3.453033
34.977324 -5.792504 3.439404
34.995107 -5.795908 3.407984
35.627432 -6.127689 2.911171
35.773060 -6.285635 3.036768
35.291991 -6.092842 3.590255
FEnd


+-+CCS_record::Boundary loops before union-find
Start boundary loop loop_id 0  init_edge IE_A_B
xyz : 48.8047 -11.7695 -8.95572
ETC
End loop
Boundary info init_edge IE_A_B [total exposed]: 199.107438 199.107438

Voronoi Facets of interface MI_AWi_BWi

MUTATIS MUTANDIS wrt interface MI_AB
```

4.3.6 File `fprefix_patches-IV.txt`

▷ **Description: Patches of the interfaces.**

Before the merge step, for each cc of the AB interface, all atoms involved in that cc are listed. Atoms involved in several cc are also reported. The same statistics are reported after the merge step for the ABW interface.

▷ **Verbatim.**

```
Patches: interface AB with 3 patches


Patch id 0
Patch size 440.30
Patch #atoms: 140
  277   CB TYR A  32
ETC


MUTATIS MUTANDIS for the remaining patches

1 atom(s) in more than 1 patch
 3135  ND2 ASN C 103


Patches: interface ABW with 1 merged patches

Merged patch id 0
Patch size 1377.64
Patch #atoms: 329
  236  ND2 ASN A  28
ETC
0 atom(s) in more than 1 patch
```

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