Voronoi diagrams for molecules

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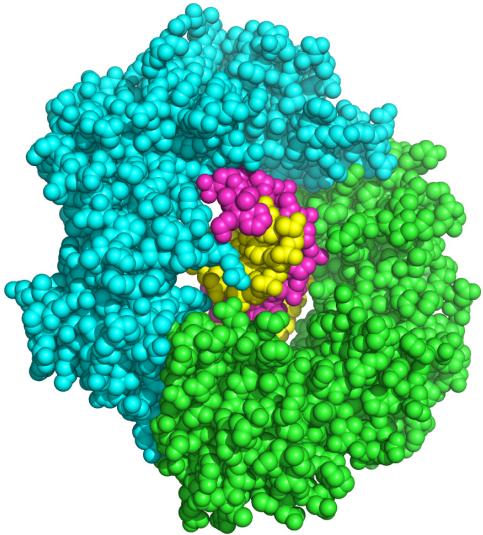
Institute of Biotechnology



When studying biological macromolecules, some common problems are:

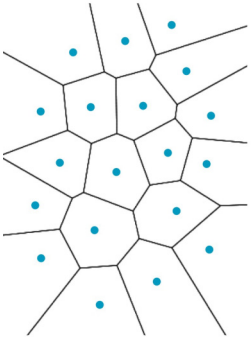
- analyzing how different parts in a molecule interact
- selecting the best prediction of a multimeric complex

Some possible solutions involve:

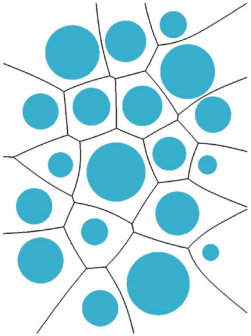
- computational geometry
- machine learning using **open data**
- developing free software

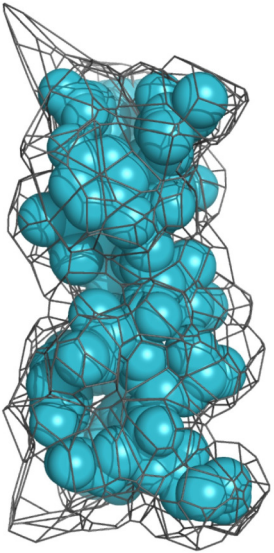
Voronoi diagram of points and balls

"Classic" Voronoi diagram of points



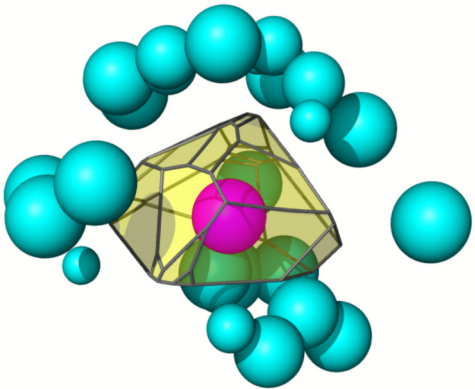
Voronoi diagram of balls



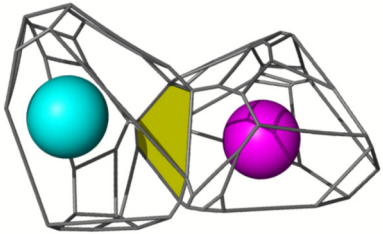


Voronoi tessellation-based analysis of structures

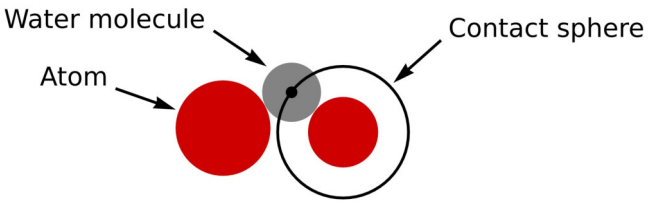
Voronoi cell of an atom surrounded by its neighbors

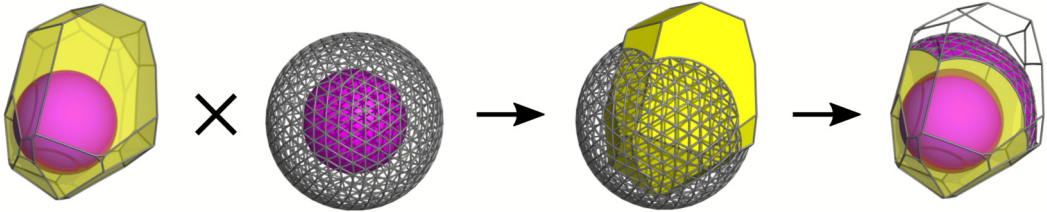


Atom-atom contact surface defined as the face shared by two adjacent Voronoi cells.



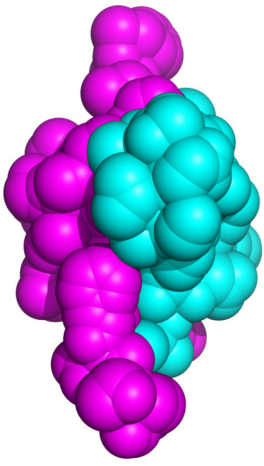
Constrained contacts



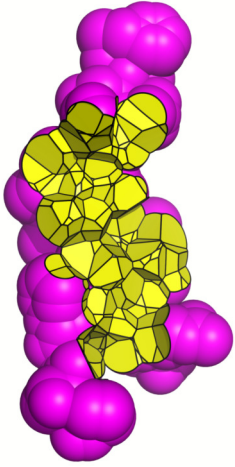


Inter-chain contacts

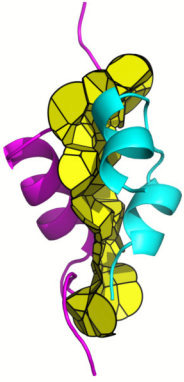
Solvent-accessible surface of an insulin heterodimer PDB:4UNG colored by subunit



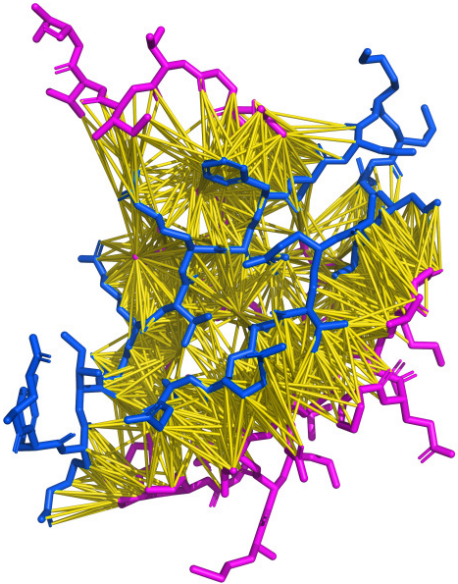
The intersubunit interface shown together with the SAS of one subunit



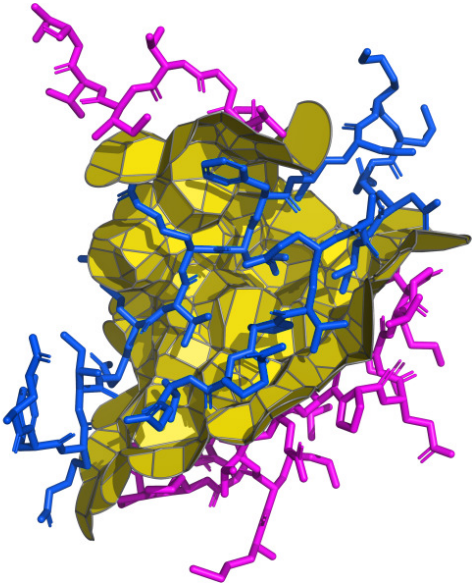
The intersubunit interface shown together with both subunits represented as cartoons



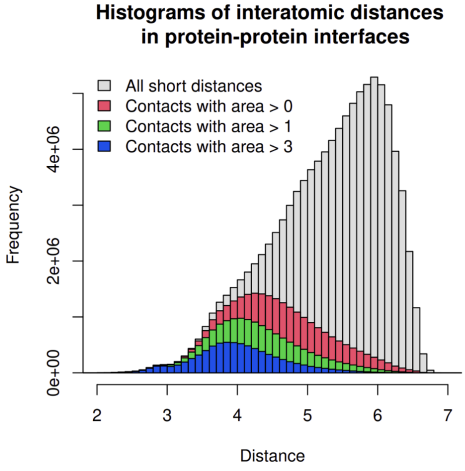
Inter-chain contact areas vs distances

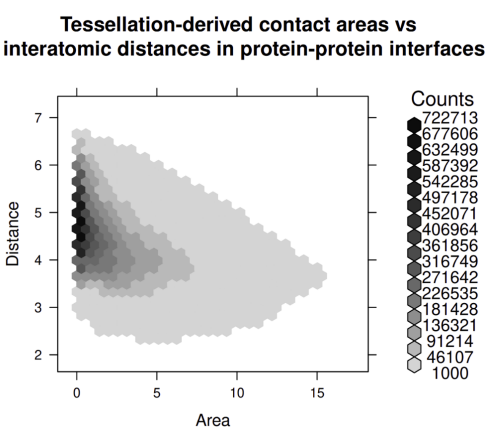


VS



Inter-chain contact areas vs distances, PDB-based statistics

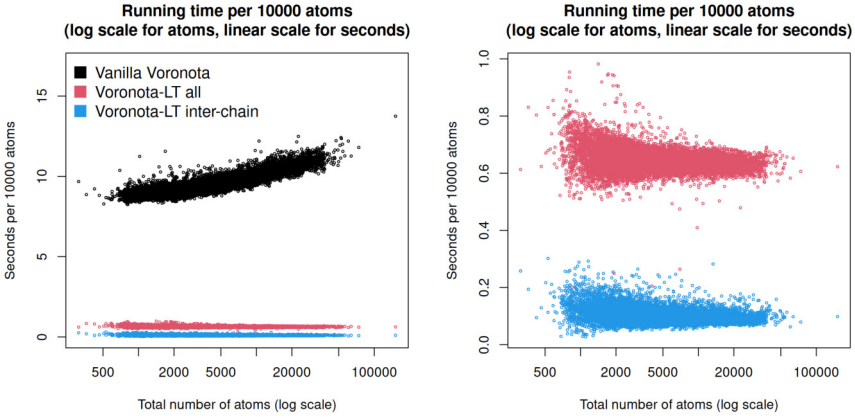




corr(area, distance) ≈ -0.43

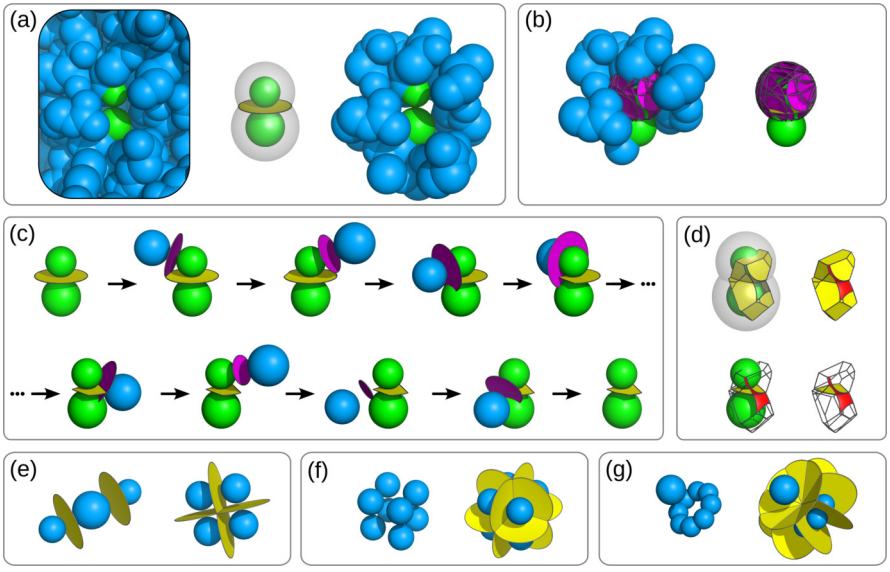
Voronota-LT

Voronota-LT is a new fast software for constructing tessellation-derived atomic contact areas and volumes. It is significantly faster than its predecessor, Voronota:



Olechnovic and Grudinin. *Voronota-LT: efficient, flexible and solvent-aware tessellation-based analysis of atomic interactions*. JCC (2025)

Voronota-LT



Getting COD crystal structure data using OPTIMADE API

```
#!/bin/bash

CODID="7250851"

JSONFILE="./optimade_cod_${CODID}.json"

[ -s "$JSONFILE" ] || \
curl -s "https://www.crystallography.net/cod/optimade/structures/${CODID}?
response_fields=cartesian_site_positions,species_at_sites,lattice_vectors,species" \
> "$JSONFILE"
```

Getting COD crystal structure data using OPTIMADE API

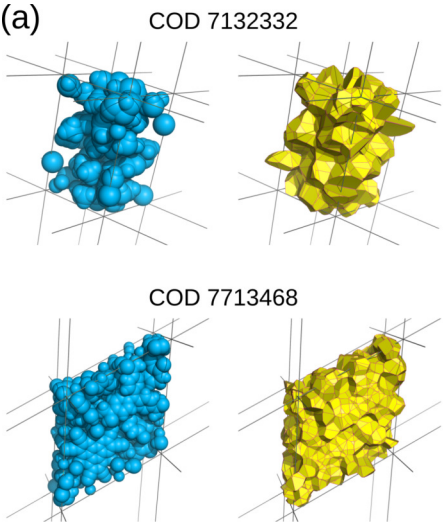
```
kliment@local:/tmp$ jq '.data.attributes.cartesian_site_positions[]' "${JSONFILE}"

[
  2.05265319791184,
  5.890757274,
  4.58437338884256
]
[
  4.39151320737323,
  13.277657274,
  3.14201180150793
]
[
  2.7797796126583,
  8.883042726,
  10.8683969918584
]
[
  0.440919603196916,
  1.496142726,
  12.310758579193
]

...
```

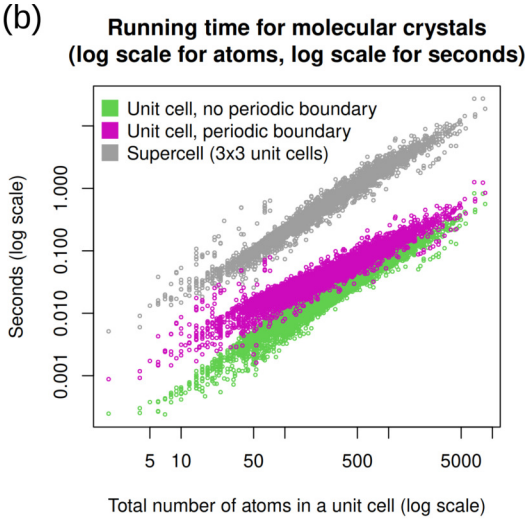
Getting COD crystal structure data using OPTIMADE API

```
kliment@local:/tmp$ jq '.data.attributes.lattice_vectors' "${JSONFILE}"
```

```
[
  [
    8.0559,
    0,
    0
  ],
  [
    0,
    14.7738,
    0
  ],
  [
    -3.22346718942986,
    0,
    15.452770380701
  ]
]
```

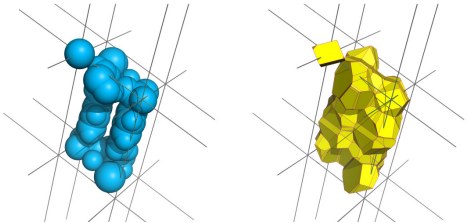
Running Voronota-LT on COD data



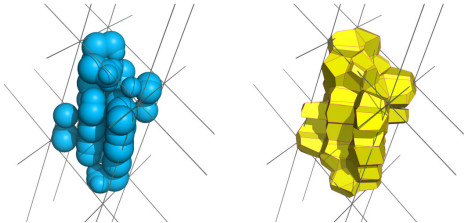


Running Voronota-LT on COD data — some examples

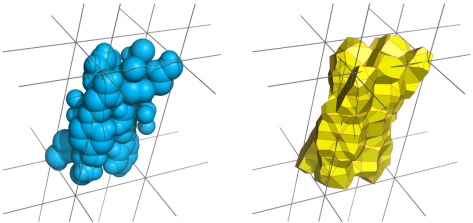
COD 7247424



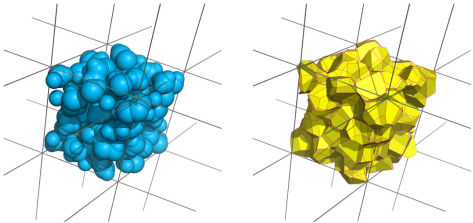
COD 7246672



COD 7132033

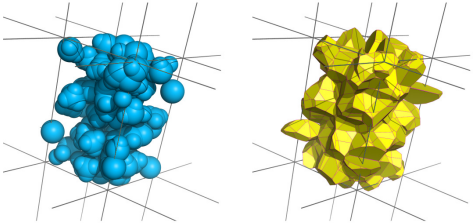


COD 7712772

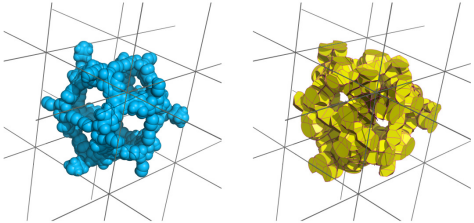


Running Voronota-LT on COD data — some examples

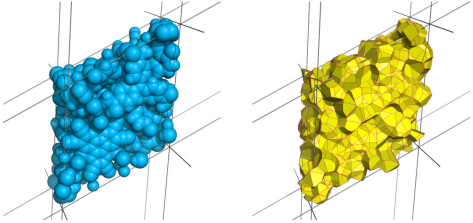
COD 7132332



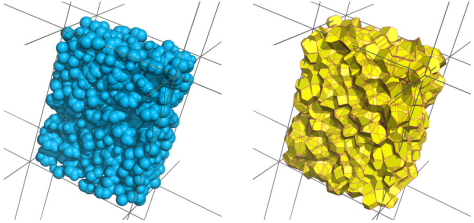
COD 7131232



COD 7713468



COD 1569733



Thanks

Thank you!

Useful links:

- https://www.kliment.lt
- https://www.bioinformatics.lt
- https://grulab.imag.fr

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