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Supplementary Material to

Extraction of Robust Voids and Pockets in Proteins

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Appendix A: Stability of pockets

The notion of stability defined for voids can be extended to pockets as well. A pocket may be destroyed in the filtration by the addition of a triangle. By destroying the pocket, this triangle creates a void, or a void-pocket pair. In our current implementation, the voids that are created by the triangle are given preference over pockets that are destroyed in the $(-\varepsilon,\varepsilon)$ range. We choose to do this because a pocket with a very narrow opening (size less than ε) will not allow any ion to pass into it, and hence functions more as a void.

Therefore, the only stable pockets that are identified correspond to those that are destroyed or split into a void-pocket pair outside of the $(-\varepsilon,\varepsilon)$ range. However, in case a pocket is preferred over a stable void, the algorithm can be easily modified to delay the insertion of the triangle that destroys the pocket, along with its coface tetrahedra.

Appendix B: Additional results

In this section, we show results obtained for proteins having PDB identifiers 4HHB and 4B87. The protein 4HHB has a total of of 72 voids, shown in Figure 1(a). Using a value of $\varepsilon = 1.0$ and further removal of voids having persistence $\pi < 0.01$ results in a total of 70 $(1.0,0.01)$-stable voids, see Figure 1(b). Figure 1(c) shows two nearby voids in the protein which merge to form a single stable void, see Figure 1(d). Note that a value of $\varepsilon = 1.0$ is equivalent to an increase / decrease of the radius of an atom by at most 0.33Å, which is within the tolerated 0.5Å used by the biologists. Modifying the filtration and computing the stable voids for this protein takes 62 secs.

Figure 2 shows the visualization of the (ε,π)-stable voids for the protein 4B87. Modifying the filtration and computing the stable voids for this protein takes 33 secs.

The implementation for now uses a naive approach of explicitly computing the voids/pockets while constructing the set of simplices which needs to be moved and thus the running time is large. This can be reduced by tracking the creators of voids/pockets as described in [ELZ02].

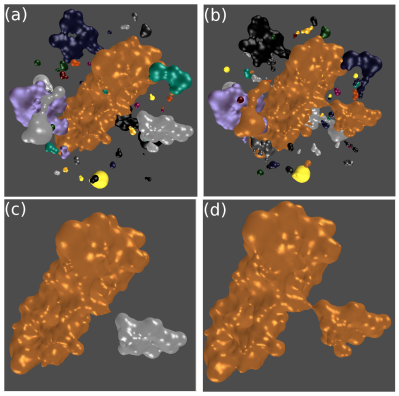


Figure 1: *Visualization of voids of the protein 4HHB. The values $\varepsilon = 1.0$ and $\pi = 0.01$ was used to compute the set of stable voids.* ***(a)*** *Voids in the protein computed at $\alpha = 0$. Number of voids = 72.* ***(b)*** *The set of $(1,0.01)$-stable voids. Number of $(1.0,0.01)$-stable voids = 70.* ***(c)*** *Two nearby voids in the protein.* ***(d)*** *These two voids merge together resulting in a single stable void.*

The variation of the number of robust voids with ε is shown in Figure 3.

Appendix C: Validation of computed cavity volumes

There is usually a variation in the volumes of cavities computed using various methods (refer [CBV02]). This variation probably arises due to the different models used for computing the volumes. Therefore, we perform an additional normalization of the computed volumes using model mutants [CBV02] to eliminate such variations. The volumes computed using our computation is normalized as follows:

$$Volume = 2.54 \times ComputedVolume + 60.77.$$

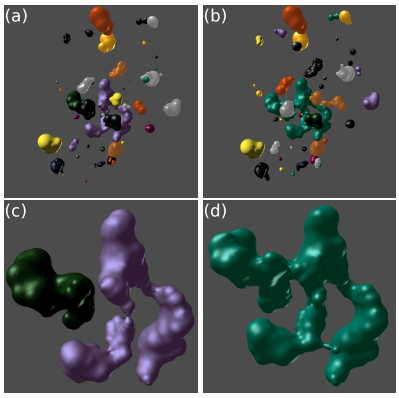
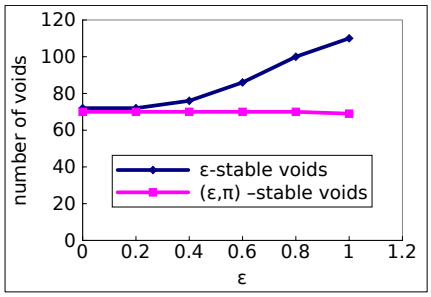
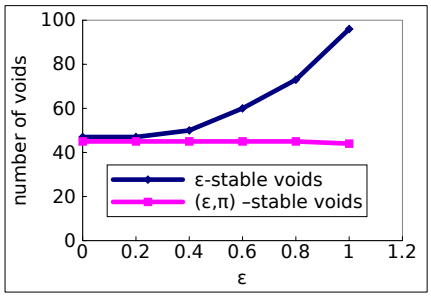


Figure 2: *Visualization of voids of the protein 4B87. The values* $\varepsilon = 1.0$ *and* $\pi = 0.01$ *was used to compute the set of stable voids.* ***(a)*** *Voids in the protein computed at* $\alpha = 0$*. Number of voids* = 47. ***(b)*** *The set of* $(1.0, 0.01)$*-stable voids. Number of* $(1.0, 0.01)$*-stable voids* = 44. ***(c)*** *Two of the nearby voids in the protein.* ***(d)*** *These voids merge together resulting in a single stable void.*



(a) Protein 4HHB



(b) Protein 4B87

Figure 3: *Graphs showing the variation of the number of voids with varying* ε*. Note that there is an increase in* ε*-stable voids as we consider a larger interval but the number of* (ε, π) *voids are less than or equal to original number of voids.*

In order to verify the correctness of the volumes computed by our software *RobustVoids*, we compare them to the volumes computed using *MC Cavity* [CBV02], see Figure 4. Note that we use normalised volumes in this graph.

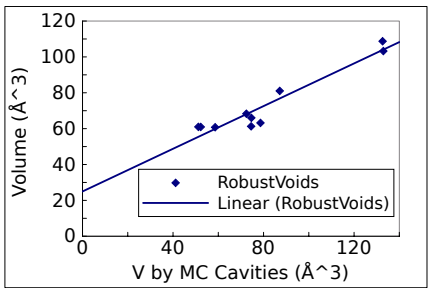


Figure 4: *Comparison of normalised volumes computed using RobustVoids and MC Cavity.*

References

[CBV02] CHAKRAVARTY S., BHINGE A., VARADARAJAN R.: A procedure for detection and quantitation of cavity volumes in proteins. *Journal of Biological Chemistry 277*, 35 (2002), 31345–31353. 1, 2

[ELZ02] EDELSBRUNNER H., LETSCHER D., ZOMORODIAN A.: Topological persistence and simplification. *Discrete & Computational Geometry 28*, 4 (2002), 511–533. 1