

# Frédéric CAZALS

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## 1 **Positions**

- 2019– Endowed chair, Interdisciplinary Institutes of Artificial Intelligence (3IA Côte d’Azur, <http://3ia.univ-cotedazur.fr/>), within the focus area *Computational Biology and Bio-Inspired AI*.
- 2016 Research Director (DR1), Algorithms-Biology-Structure, Inria Sophia Antipolis.
- 2007– Group leader, Algorithms-Biology-Structure, Inria Sophia Antipolis.
- 2006 Research Director (DR2), Geometrica group, Inria Sophia Antipolis.
- 2000 Tenured researcher and CR1 promotion, Prisme group, Inria Sophia Antipolis.
- 1998-00 Researcher (CR2) in the Prisme group, Inria Sophia Antipolis.

## 2 **Education**

- 2006: *Habilitation*, University of Nice Sophia Antipolis. Title: “*Computational Geometry and Topology: Concepts, Algorithms, Applications*”.
- 1998: Post-Doc at Inria Sophia Antipolis, France, Prisme project.(Head: Jean-Daniel Boissonnat.)
- 1997: Post-Doc at Inria Rocquencourt, France, Algorithms project. Head: Philippe Flajolet.
- 1995-96: National Service, Robotics Laboratory, Stanford University (USA), with a financial support from Matra Datavision (France). Head: Jean-Claude Latombe.
- 1996-97,93-95: PhD in Theoretical Computer Science, University of Paris VII. Title: “*Structures de données hiérarchiques non récursives et problèmes de proximité*”. Advisor: Claude Puech. Grade: Lab: iMAGIS-IMAG (Grenoble, France). Congratulations of the Committee.
- 1991-92: Diplôme d’Etudes Approfondies in Computer Science at the Ecole Normale Supérieure, Ecole Polytechnique and University of Paris VII in (Paris, France). With distinction.
- 1989-92: Institut National Agronomique Paris-Grignon (Paris, France), the most selective engineering high school in biological and mathematical sciences.
- 1987-89: A two years examination preparation for high schools in biological and mathematical sciences.
- 1987: *Baccalauréat* in Science, with highest distinctions.

## 3 **Visiting positions**

*Indian Institute of Technology of Kanpur*, N Rama Rao Professor in CSE, Jan.-Feb. 01.

*Stanford University*, Robotics Lab. From the 03/01/95 to the 05/31/96. Visiting scholar.

## 4 **Supervision of students and postdocs**

### Postdocs.

- D. Mazauric, January 2015 - September 2015. PhD in Computer Science.  
Topic: *Comparing biomolecular energy landscapes*.  
Publications: [18, 77].  
*Early job*: research scientist at Inria, ABS project-team.

- N. Malod-Dognin, July 2010 - June 2012. PhD in Computer Science.  
Topic: *Modeling and comparing protein binding patches*.  
Publications: [68, 47].  
*Early job*: post-doctoral research associate, department of computing, Imperial College London.
- S. Lorient, December 2008 - November 2009. PhD in Computer Science.  
Topic: *Robust software for molecular modeling*.  
Publications: [74, 25, 43].  
*Early job*: software engineer with the Geometry factory (<http://geometryfactory.com/>).
- B. Bouvier, November 2006 - April 2008, PhD in Biophysics.  
Topic: *Modeling the flexibility of proteins*.  
Publication: [8].  
*Early job*: research scientist at CNRS.
- F. Proust, November 2004 - October 2005, PhD in Biochemistry.  
Topic: *Modeling protein - protein interfaces*.  
Publication: [33].  
*Early job*: software engineer with La banque postale.

#### PhD students: ongoing.

- M. Simsir, 2018-20. *Structural modeling of multidrug resistance transporters in cancer* NB: co-advised with I. Mus-Veteau, IPMC/CNRS.  
Publication(s): [51].
- T. O'Donnell, 2018-2010. *Modeling the influenza polymerase: methods and applications*  
Nb: co-advised with B. Delmas, INRAe.  
Publication(s): [76].

#### PhD students: suspended.

- C. Roth, 2010-... *Biomolecular energy landscapes: sampling and characterization*  
Publications: [18, 50] Status of the thesis, as of December 2015: suspended for startup creation.

#### PhD students: defended.

- A. Chevallier, 2015-19. *Random walks for estimating the volume of convex bodies and densities of states in high dimensional spaces*  
Committee: T. Lelièvre (Ecole des Ponts et Chaussees, reviewer), D. Wales (Cambridge university, reviewer), J-D. Boissonnat (Inria), C. Robert (CNRS / IBPC), A. Trouné (ENS Paris-Saclay), F. Cazals (Inria). Publications: [36, 80, 79]  
*Early job*: post-doc, Univ. of Lancaster.
- R. Tetley, 2014-18. *Mixed sequence-structure based analysis of proteins, with applications to functional annotations*  
Committee: J. Cortés (CNRS, reviewer), J-F. Gibrat (INRA, reviewer), M. Weigt, Professeur (Sorbonne University), F. Rey, Professeur (CNRS, Inst. Pasteur Paris, French Academy of Sciences), D. Mazauric (Inria), F. Cazals (Inria).  
Publications: [29, 35, 78, 81]  
*Early job*: startup founder.
- S. Marillet, 2013-16. *Modeling the antibody response: from the structure of immunoglobulins - antigen complexes to the clonal complexity of heavy chain repertoires*

Thesis is co-advised with P. Boudinot (INRA Jouy-en-Josas). Committee: P. Bates (Francis Crick Institute, reviewer), A. Bonvin (Utrecht University, reviewer), D. Housset (CEA), V. Braud (CNRS), P. Boudinot (INRA), F. Cazals (Inria). Publications: [48, 49, 40].

*Early job:* research engineer at the Poitiers CHU Hospital.

- A. Lhéritier, 2011-15. *Nonparametric methods for learning and detecting multivariate statistical dissimilarity* Committee: G. Seroussi (Univ. de la République, Uruguay), P. Grünwald, CWI, Netherland), G. Obozinski Chercheur (Ecole des Ponts ParisTech), V. Zarzoso (Univ. de Nice Sophia Antipolis), F. Cazals (Inria).  
Publications: [66, 42, 73].  
*Early job:* data scientist with Amadeus (<http://www.amadeus.com>).
- D. Agarwal, 2011-15. *Topics in mass spectrometry based structure determination* Committee: P. Barran (Univ. Manchester), R. Andonin (Univ. Rennes), J. Chamot-Rooke (Inst. Pasteur Paris), G. Bernot (Univ. Nice), F. Cazals (Inria Sophia Antipolis).  
Publications: [4, 53, 82].  
*Early job:* postdoc at the Harvard Medical school.
- T. Dreyfus, 2008-10. *Assessing the Reconstruction of Macro-molecular Assemblies: the Example of the Nuclear Pore Complex* Committee: J. Giesen (Jena Univ., Germany), P. Schultz (IGBMC Strasbourg/CNRS), G. Bernot (Univ. of Nice, France), J.-D. Boissonnat (Inria Sophia Antipolis), A. Denise (Univ. of Orsay), F. Rey (CNRS, Inst. Pasteur Paris, French Academy of Sciences), F. Cazals (Inria Sophia Antipolis).  
Publications: [63, 37, 19].  
*Early job:* research engineer at Inria, then self-employed, then Google Zurich (March 2019).
- S. Lorient, 2005-08. *Arrangements of Circles on a Sphere: Algorithms and Applications to molecular models represented by union of balls* Co-advised with F. Chazal. Committee: R. Lavery (CNRS, France), J. Snoeyink (UNC, USA), J. Maddocks (EPFL, Switzerland), R. Roussarie (Univ. Bourgogne, France), F. Chazal (Inria Saclay), F. Cazals (Inria Sophia Antipolis).  
Publications: [67, 10, 28, 45].  
*Early job:* software engineer with the Geometry factory (<http://geometryfactory.com/>).
- M. Pouget, 2002-05. *Geometry of surfaces: from the estimation of local differential quantities to the robust extraction of global differential features* Committee: N. Ayache (Inria), P. Giblin (Liverpool), J.-M. Morvan (Lyon), S. Petijean (Inria Nancy), K. Polthier (Berlin), J.-P. Thirion (Quantificare), F. Cazals (Inria, advisor).  
Publications: [31, 30, 87, 21, 22].  
*Early job:* research scientist with Inria.

## Master students.

- T. O'Donnell, summer 2018. *Structural modeling of FMRP dimers in solution.*
- N. Gayraud, summer 2015. *Detecting secondary structure elements in cryo electron microscopy maps, with applications to coarse grain model reconstruction.*
- R. Tetley, Master in computer science, ENS Lyon, summer 2014. *Beyond rigid structural alignments, with applications in structural virology.*
- T. Dreyfus, Master in Bioinformatics from the Univ. of Orsay - Paris XI, summer 2008. *Reconstructing large macro-molecular assemblies.*
- S. Lorient, Master interm from Univ. of Bourgogne at Dijon, summer 2005. *Exact arrangements of circles on spheres.*  
Publication: [67]

- J. Flototto, Master intern from Univ. Nice Sophia Antipolis, summer 1999. *Automatic drawing of similar molecules.*  
Publication: [57]

### Summer interns.

- G. Sales Santa Cruz, intern from Polytech Nice, summer 2019. *Source-target interpolation in protein protein interaction networks.* Co-advised with D. Mazaauric.
- M. Guramare, intern from Harvard university, summers 2018 and 2019. *Sequence alignment algorithms with topological constraints.* Co-advised with D. Mazaauric.
- P. Shah, intern from IIT Bombay, summer 2011. *Geometric optimization problems for collections of balls.*  
Publication: [20].
- A. Bansal, intern from IIT Bombay, summer 2010. *On the Morphology of Protein Binding Patches.*  
Publication: [47].
- H. Kanhere, intern from IIT Bombay, summer 2009. *On the volume of unions of balls.*  
Publication: [25].
- N. Shah, intern from IIT Bombay, summer 2009. *Geometric optimization algorithms for collections of balls.*  
Publication: [20]. (Curriculum: PhD student, Carnegie Mellon Univ.)
- A. Ramdas, intern from IIT Bombay, summer 2008. *Landmark based dimensionality reduction.*
- S. Sachdeva, intern from IIT Bombay, summer 2007. *Selection of diverse conformational ensembles.*  
Publication: [45].  
(Curriculum: PhD student, Princeton Univ.)
- A. Parameswaran, intern from IIT Bombay, summer 2006. *Robust construction of the extended three-dimensional flow complex.*  
Publication: [69].  
(Curriculum: PhD thesis, Stanford Univ; Professor, University of Illinois at Urbana Champaign)
- C. Karande, intern from IIT Bombay, summer 2005. *Partial combinatorial shape matching.*  
Publications: [26, 27]  
(Curriculum: PhD thesis at Georgia Tech. Now with Google research.)
- P. Agrawal, intern from IIT Bombay, summer 2004. *Partial shape matching.*  
(Curriculum: PhD thesis at Stanford Univ.)
- K. Chaudhuri and S. Saha, interns from IIT Kanpur, summer 2001. *Local Approximation of Triangulated Surfaces.* (Curriculum: K. Chaudhuri, PhD at Berkeley Univ.; Prof. at UCSD)
- S. Srivastava, intern from IIT Kanpur, summer 2000. *From triangulated surfaces to primitive surfaces.*  
(Curriculum: PhD, Univ. of Massachusetts, Amherst.)

## 5 Courses, schools, conferences

### 5.1 Courses

#### Master program coordination

- 2018–: member of the steering committee of the Master of Science Quantitative and computational sciences for biomedical data – <http://univ-cotedazur.fr/education/training?AICAL18&lang=en#.XEYJYcZ71mM>
- 2009-11, Program coordinator of the **Master of Science in Computational Biology**, Univ. of Nice Sophia Antipolis (<http://www.computationalbiology.eu>). Together with Pierre Kornprobst (Inria Sophia), we launched and administrated for two years this international master program.

#### Courses taught: current courses

Regular courses:

- 2014–... , *Foundations of Geometric Methods in Data Analysis* (<ftp://ftp-sop.inria.fr/abs/fcazals/classes/centrale-G0uDA.html>), Data Sciences Program, Department of Applied Mathematics, Ecole Centrale-Supélec (<http://cvn.ecp.fr/teaching/data-sciences/>). Course taught with F. Chazal, from Inria Saclay.
- 2009–2016, *Algorithmic problems in computational structural biology*, University of Nice - Sophia Antipolis, Master of Science in Computational Biology, FC (24h).

Mini-courses:

- Computational structural biology: a primer. Ecole GDR Bioinformatique moléculaire, Frejus, June 2018.
- Nearest Neighbors Algorithms in Euclidean and Metric Spaces: Algorithms and Data Structures, F. Cazals. Winter school Computational Geometry and Topology for Data Analysis, Inria Sophia Antipolis, January 2017.
- Algorithms for characterizing and comparing samplings of potential energy surfaces, F. Cazals and C. Robert. Winter School Algorithms in Structural Bio-informatics, Cargese, December 2015.
- Geometric methods in data analysis, F. Cazals and S. Oudot. Summer School Biomedical Image Analysis Summer, Paris, July 6-10, 2015.
- Modeling Contacts in Macro-molecular assemblies: from Inference to Assessment, F. Cazals. Winter School Algorithms in Structural Bio-informatics, Inria Sophia Antipolis, December 2014.
- Analyzing conformational landscapes, with applications to the design of collective coordinates, F. Cazals and C. Robert. Winter School Algorithms in Structural Bio-informatics, Toulouse, November 2013.
- Modeling Macro-Molecular Complexes and Assemblies, F. Cazals. Athens University – invited Mini-course, May 2013.
- Modeling protein complexes and assemblies with Voronoi diagrams, F. Cazals. Winter School Algorithms in Structural Bio-informatics, Inria Sophia Antipolis, December 2012. Web: <http://www-sop.inria.fr/manifestations/algoSB/>.

## Courses taught: past courses (last five years)

- 2010-2014, *Geometric and topological modeling with applications in biophysics*, Ecole Centrale Paris, Master degree in applied mathematics. FC (24h).
- 2007-10, *Algorithmic Problems in Structural Biology*, Orsay University. FC (12h), J. Janin, Orsay (6h) and C. Robert, CNRS (6h). NB: This course was offered to students from 3 masters: *Bioinformatique*, *Mathématiques*, *Innovation Thérapeutique*.

## 5.2 Conferences and workshops

### 5.2.1 Summer / Winter schools

**Winter school Algorithms in Structural Biology.** Together with J. Cortés (LAAS/CNRS, Toulouse), and C. Robert (IBPC/CNRS, Paris), we launched and have been organizing the the Winter Schools series *Algorithms in Structural Bio-informatics*. These schools are meant to train PhD students and post-docs on advanced algorithmic techniques in structural biology. The series goes as follows:

- 2015: Cargèse: focus on *Sampling bio-molecular systems*. Web: <http://algosb.galaxy.ibpc.fr/>
- 2014, Inria Sophia: focus on *Modeling large macromolecular assemblies*. Web: <http://algosb2014.inria.fr>
- 2013, Toulouse: focus on *Modeling the flexibility of proteins*. Web: <http://algosb.sciencesconf.org/>
- 2012, Inria Sophia: focus on *Modeling protein - protein interactions*. Web: <http://www-sop.inria.fr/manifestations/algoSB/>

High profile classes are offered, and the series encounters a frank success: for the previous editions,  $\sim 40$  attendees from top labs around the world participated.

**Statistical Learning Theory: a Short Course, by P. Grünwald.** In June 2013, I organized in Sophia-Antipolis a minicourse on statistical learning theory, a topic of interest for six project teams from Inria Sophia. The details can be found at <https://team.inria.fr/abs/statistical-learning-theory-a-short-course/>.

### 5.2.2 Conferences

**Energy Landscapes 2016.** In 2016, together with J. Cortés (LAAS/CNRS, Toulouse), and C. Robert (IBPC/CNRS, Paris), we organize the international conference on *Energy Landscapes* (<http://eland2016.inria.fr/>), the premier meeting for scientists (physicists, chemical physicists, bio-physicists, biologists, computer scientists) working on the problem of computing (potential, free) energies for bio-molecular systems.

The previous editions were organized in Durham, UK (2014; <https://www.dur.ac.uk/soft.matter/events/energylandscapes/>), Telluride, US (2013, 2015; <http://www.telluridescience.org/meetings/workshop-details?wid=547>), and Obergurgul, Austria (2012, <http://www.esf.org/?id=9134>).

**ALGO 2013.** I have been a member of the organization committee of the premier federated conference on algorithm in Europe, ALGO'2013 (<http://algo2013.inria.fr>). The venue involved seven international conferences, for circa 450 attendees.

## 6 **Publications**

## 7 **Books**

- [1] F. Cazals and P. Kornprobst, editors. *Modeling in Computational Biology and Medicine: A Multidisciplinary Endeavor*. Springer, 2013.

## 8 **Thesis**

- [2] F. Cazals. *Structures de données hiérarchiques non récursives et problèmes de proximité*. Phd thesis (thèse de doctorat), Univ. Paris VII, France, 1997.
- [3] F. Cazals. *Computational Geometry and Topology: Concepts, Algorithms, Applications*. Habilitation, Univ. Nice Sophia Antipolis, France, 2006.

## 9 **Journals and book chapters**

- [4] D. Agarwal, C. Caillouet, D. Coudert, and F. Cazals. Unveiling contacts within macro-molecular assemblies by solving minimum weight connectivity inference problems. *Molecular and Cellular Proteomics*, 14:2274–2282, 2015.
- [5] J.-D. Boissonnat and F. Cazals. Natural coordinates of points on a surface. *Computational Geometry Theory and Applications*, 19(2):155–173, 2001.
- [6] J.-D. Boissonnat and F. Cazals. Smooth surface reconstruction via natural neighbour interpolation of distance functions. *Computational Geometry Theory and Applications*, 22(1):185–203, 2002. Conf. version: ACM Sympos. Comput. Geom. '00.
- [7] V. Borrelli, F. Cazals, and J.-M. Morvan. On the angular defect of triangulations and the pointwise approximation of curvatures. *Computer Aided Geometric Design*, 20(6):319–341, 2003.
- [8] B. Bouvier, R. Grunberg, M. Nilgès, and F. Cazals. Shelling the Voronoi interface of protein-protein complexes reveals patterns of residue conservation, dynamics and composition. *Proteins: structure, function, and bioinformatics*, 76(3):677–692, 2009.
- [9] J. Carr, D. Mazauric, F. Cazals, and D. J. Wales. Energy landscapes and persistent minima. *The Journal of Chemical Physics*, 144(5):4, 2016.
- [10] P. M. M. De Castro, F. Cazals, S. Lorient, and M. Teillaud. Design of the cgal spherical kernel and application to arrangements of circles on a sphere. *Computational Geometry: Theory and Applications*, 42(6-7):536–550, 2009.
- [11] R. Castro, L. Journeau, H.P. Pham, O. Bouchez, V. Giudicelli, M.-P. Lefranc, E. Quillet, A. Benmansour, F. Cazals, A. Six, S. Fillatreau, O. Sunyer, and P. Boudinot. Teleost fish mount complex clonal IgM and IgT responses in spleen upon systemic viral infection. *PLOS Pathogens*, 9(1):e1003098, 2013.
- [12] F. Cazals. Combinatorial properties of one-dimensional arrangements. *Experimental Mathematics*, 6(1):87–94, 1997.
- [13] F. Cazals. Data structures and basic algorithms. In P. Frey and P.-L. George, editors, *Mesh Generation. Application to finite elements*. Oxford, 2000.
- [14] F. Cazals. Non-intrusive debugging and incremental visualization with the geometric stethoscope. *J. of Graphics Tools*, 7(2):27–40, 2002.



- [15] F. Cazals, F. Chazal, and J. Giesen. Spectral Techniques to Explore Point Clouds in Euclidean Space, with Applications to Collective Coordinates in Structural Biology. In Ioannis Z. Emiris, Frank Sottile, and Thorsten Theobald, editors, *Nonlinear Computational Geometry*, volume 151 of *The IMA Volumes in Mathematics and its Applications*, pages 1–34. Springer, 2010.
- [16] F. Cazals and D. Cohen-Steiner. Reconstructing 3D compact sets. *Computational Geometry Theory and Applications*, 45(1-2):1–13, 2011.
- [17] F. Cazals and T. Dreyfus. The Structural Bioinformatics Library: modeling in biomolecular science and beyond. *Bioinformatics*, 7(33):1–8, 2017.
- [18] F. Cazals, T. Dreyfus, D. Mazauric, A. Roth, and C.H. Robert. Conformational ensembles and sampled energy landscapes: Analysis and comparison. *J. Comp. Chem.*, 36(16):1213–1231, 2015.
- [19] F. Cazals, T. Dreyfus, and C.H. Robert. Modeling macro-molecular complexes : a journey across scales. In F. Cazals and P. Kornprobst, editors, *Modeling in Computational Biology and Medicine: : A Multidisciplinary Endeavor*. Springer, 2013.
- [20] F. Cazals, T. Dreyfus, S. Sachdeva, and N. Shah. Greedy geometric algorithms for collections of balls, with applications to geometric approximation and molecular coarse-graining. *Computer Graphics Forum*, 33(6):1–17, 2014.
- [21] F. Cazals, J.-C. Faugère, M. Pouget, and F. Rouillier. The implicit structure of ridges of a smooth parametric surface. *Computer Aided Geometric Design*, 23(7):582–598, 2006.
- [22] F. Cazals, J.-C. Faugère, M. Pouget, and F. Rouillier. Ridges and umbilics of polynomial parametric surfaces. In B. Juettler and R. Piene, editors, *Computational Methods for Algebraic Spline Surfaces II*, pages 141–159. Springer, 2006.
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- [24] F. Cazals, J. Giesen, M. Pauly, and A. Zomorodian. The conformal alpha shapes filtration. *The Visual Computer*, 22(8):531–540, 2006.
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- [26] F. Cazals and C. Karande. An algorithm for reporting maximal  $c$ -cliques. *Theoretical Computer Science*, 349(3):484–490, 2005.
- [27] F. Cazals and C. Karande. A note on the problem of reporting maximal cliques. *Theoretical Computer Science*, 407(1–3):564–568, 2008.
- [28] F. Cazals and S. Lorient. Computing the exact arrangement of circles on a sphere, with applications in structural biology. *Computational Geometry: Theory and Applications*, 42(6-7):551–565, 2009.
- [29] F. Cazals, D. Mazauric, R. Tetley, and R. Watrigant. Comparing two clusterings using matchings between clusters of clusters. *ACM J. of Experimental Algorithms*, 24(1):1–42, 2019.
- [30] F. Cazals and M. Pouget. Differential topology and geometry of smooth embedded surfaces: selected topics. *Int. J. of Computational Geometry and Applications*, 15(5):511–536, 2005.
- [31] F. Cazals and M. Pouget. Estimating differential quantities using polynomial fitting of osculating jets. *Computer Aided Geometric Design*, 22(2):121–146, 2005.

- [32] F. Cazals and M. Pouget. Algorithm 889: Jet.fitting.3—a generic c++ package for estimating the differential properties on sampled surfaces via polynomial fitting. *ACM Transactions on Mathematical Software*, 35(3):24, 2008.
- [33] F. Cazals, F. Proust, R. Bahadur, and J. Janin. Revisiting the Voronoi description of protein-protein interfaces. *Protein Science*, 15(9):2082–2092, 2006.
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- [35] F. Cazals and R. Tetley. Characterizing molecular flexibility by combining IRMSD measures. *Proteins: structure, function, and bioinformatics*, 87(5):380–389, 2019.
- [36] A. Chevallier and F. Cazals. Wang-Landau algorithm: an adapted random walk to boost convergence. *J. of Computational Physics*, NA(NA), 2020.
- [37] T. Dreyfus, V. Doye, and F. Cazals. Assessing the reconstruction of macro-molecular assemblies with toleranced models. *Proteins: structure, function, and bioinformatics*, 80(9):2125–2136, 2012.
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## 10 Conferences

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## 11 Submitted

- [75] S. Bereux, B. Delmas, and F. Cazals. Boosting the analysis of protein interfaces with multiple interface string alignment: illustration on the spikes of coronaviruses. *Submitted*, 2020.
- [76] F. Cazals, B. Delmas, and T. O’Donnell. Fréchet mean and  $p$ -mean on the unit circle: characterization and algorithm. *Submitted*, 2020.
- [77] F. Cazals and D. Mazauric. Optimal transportation problems with connectivity constraints. Research Report 8991, Inria Sophia Antipolis ; Université Côte d’Azur, 2016. Submitted.
- [78] F. Cazals and R. Tetley. Multiscale analysis of structurally conserved motifs. *Submitted*, 2020. Submitted.
- [79] A. Chevallier and F. Cazals. A generic framework for Wang-Landau type algorithms. *Submitted*, 2020.

- [80] A. Chevallier, S. Pion, and F. Cazals. Hamiltonian monte carlo with boundary reflections, and application to polytope volume calculations. *Submitted*, 2018.
- [81] R. Tetley, J. Fedry, P. Guardado-Calvo, F. Rey, and F. Cazals. Hybrid sequence-structure based hmm models leverage the identification of homologous proteins: the example of class II fusion proteins. *Submitted*, 2019.

## 12 Misc

- [82] D. Agarwal, F. Cazals, and N. Malod-Dognin. Stoichiometry determination for mass-spectrometry data: the interval case. Technical Report 8101, Inria, 2014.
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- [85] F. Cazals. La morphologie des contacts entre bio-molécules. *Pour la Science*, Juillet - Août:44–48, 2006.
- [86] F. Cazals, C. Mueller, C. Robert, and C.A. Roth. Towards Morse theory for point cloud data. Technical Report 8331, Inria, 2013.
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- [89] D. Mazauric. *Graphes et Algorithmes – Jeux grandeur nature*. Inria, 2016.

## 13 Recent invited talks

- *Clustering algorithms for structural studies: insights on novel metrics and cluster stability assessment*, Algorithms for integrative structural biology, Grenoble, March 2020.
- *Source-Target proximity analysis in protein networks using random walks with restart; applications to cancer drug resistance prediction from single-cell data*. SOPH.I.A Summit 2019, Sophia Antipolis, December 2019.
- *Multiscale molecular flexibility analysis: novel insights*. MPI Frankfurt, July 2019.
- *Multiscale molecular flexibility analysis: novel insights*. Conference of the Polish Bioinformatics Society, Torun, June 2019.
- *Bio-molecules: on the role of geometry in the tryptic structure - dynamics -function*. Meeting of the French Academy of Sciences, French Riviera, June 2019.
- *Leveraging structural data by decoupling structure, thermodynamics and dynamics*, Challenges in large scale biomolecular simulation, Inst. Etudes Sc. de Cargese, France, May 2019
- *Mining molecular flexibility: novel tools, novel insights*, University College, London, April 2019.
- *Novel structural parameters of IG-Ag complexes yield a quantitative description of interaction specificity and binding affinity*, Journées scientifiques de la SFHI (Soc. Fr. d’histocompatibilité et d’immunogénétique), Paris, Mars 2019.
- *Energy landscapes: sampling, analysis, comparison*, RNA Kinetics days, Ecole polytechnique, October 2018.
- *Randomized algorithms for volume/density of states calculations in high-dimensional spaces*: Energy landscapes, Kalamata, Greece, September 2018; Advances in Computational Statistical Physics, CIRM, France, September 2018.

- *Understanding scoring/energy landscapes: a tale of local minima and density of states*, Meet-U: when proteins meet each other, January 2018, Paris.
- *Beyond two-sample-tests: localizing data discrepancies in high-dimensional spaces*, NIPS workshop of Topological Data Analysis, Los Angeles, December 2017.
- *Modèles géométriques pour la prédiction des interactions macro-moléculaires*, seminar for the course *Géométrie algorithmique Données, Modèles, Programmes*, by Jean-Daniel Boissonnat, Chaire d'informatique et sciences numériques, Collège de France, March 2017.
- *Modeling in structural bioinformatics: the tryptic structure - dynamics - function*, GDR Bioinformatique moléculaire, Paris, November 2017.
- *Energy landscapes: sampling, analysis*, Structural biology meets biophysics, Obernai. December 2016.
- *Modeling energy landscapes of biomolecular systems*, Ecole Normale Supérieure de Cachan. September 2016.
- *Energy landscapes: sampling, analysis, and comparison*, Energy Landscapes Workshop, Porquerolles. July 2016.
- *Novel structural parameters of IG-Ag complexes yield a quantitative description of interaction specificity and binding affinity*, Structural Aspects of Infectious Disease, Cambridge, UK, August 2016.
- *Improved understanding of protein dynamics via energy landscape sampling, analysis, and comparison*, TSRC on protein dynamics. Les Houches, March 2016.
- *Energy Landscapes: Sampling, Analysis, and Comparison*, Max-Planck Institute for Solid State Research, Stuttgart, Germany. November 2015.
- *Beyond Two-sample-tests: Localizing Data Discrepancies in High-dimensional Spaces* GUDHI workshop on topological data analysis, Porquerolles, France. October 2015.
- *Exploring and modeling energy landscapes*, University Chemical Laboratories, Cambridge University, UK. February 2015.
- *Modeling Noisy Data, with Applications in Structural Biology*, University of Athens, May 2013.
- *Stoichiometry Determination for Mass-spectrometry Data in Structural Proteomics*, Meeting of the French Biophysical Society, Grenoble, France, 2012.
- *Multiscale Analysis of Energy Landscapes based on Discrete Morse-Smale Decompositions and Bifurcations Diagrams*, Energy Landscapes Workshop (Conference from the European Science Foundation), Obergurgl, Austria, July 2012.
- *Modeling Noisy Data : Towards a Generic Framework Coupling Morse Theory and Persistence Theory*, Google Technical Talk, Google, CA, March 2012. YouTube video at <http://www.youtube.com/watch?v=JbQT0uHZnc>
- *Assessing the stability of protein complexes within large assemblies: the example of the Nuclear Pore Complex*:
  - Workshop on *Computational Challenges in Structural Biology*, Strasbourg, France, 2012.
  - International Biophysical Congress, Beijing, China, November 2011.
  - Institute of Physics, Chinese Academy of Sciences, China, November 2011.
  - Theoretical approaches for the genomes and the proteins, Laboratoire de Physique Théorique (LAPTH), Annecy, September 2011.
  - EMBO Symposium on Molecular Perspectives on Protein-Protein Interactions, Sant Feliu de Guixols, Spain, November 2010.
  - XXIIème Congrès de la Société Française de Biophysique, La-Colle-sur-Loup, September 2010.
- *Mining biophysical properties through the prism of geometry: how do forces constrain macro-molecular morphology?*, Indian Institute of Science, Bangalore, October 2011.
- *Balls, sticks, triangles and molecules*, closing workshop of the ANR Triangles, Sophia-Antipolis, December 2010.
- *Analyzing Sampled Energy Landscapes with Applications to the Design of Collective Coordinates*, CECAM workshop on the Dynamics and Thermodynamics of Biomolecular Recognition, Ecole Polytechnique, France, May 2011.

- *Geometric Models for the Description of 3D Molecular Systems*, Energy Landscapes Workshop, Chemnitz, June 2010.
- *Geometric Models for the Description of High-dimensional Point Cloud Data*, Energy Landscapes Workshop, Chemnitz, June 2010.
- *Modeling the interface of protein - protein complexes: shelling the Voronoi interface reveals patterns of composition, residue conservation, and water dynamics*, IBMC Strasbourg, Architecture et reactivite de l'ARN, May 2010.
- *Modeling water traffic at protein interfaces: from Voronoi models to (simple) percolation on lattices*, Ecole Normale Supérieure, groupe de travail Probabilités et Statistiques, April 2010.
- *Geometric techniques for the inference and the assessment of macro-molecular complexes*, IGBMC Strasbourg, September 2009.
- *Geometric representations of protein complexes and assemblies: an excursion across scales*, NIH Bethesda, NIH - Inria meeting, June 2009.
- *Models and algorithms for the description of macro-molecular interactions*, Workshop Industry Challenges in Geometric Modeling, CAD, and Simulation; Darmstadt, March 2009.
- *When Geometry meets biophysics: description of protein-protein interfaces, and selection of diverse conformational ensembles*, Sanofi-Aventis, research seminar, 12/08.
- *On the Characterization of Diverse Conformational Ensembles, with Applications to Flexible Docking*; Approximation, Modélisation Géométrique et Applications, CIRM Marseille, 11/08.
- *Modeling protein - protein interactions: the geometry of active residues and the selection of conformers*; IRISA, Rennes, 05/2008.
- *Protein folding: energy landscapes, spectral analysis, and Morse theory*; Journées de Dynamique Non Linéaire, Marseille; 01/08.
- *Describing protein-protein and atomic environments: a geometric perspective*; (i) Dpts of Biopharmaceutical Sciences and Pharmaceutical Chemistry (SALILAB), UCSF, 11/07; (ii) Dpt of Structural Biology, Stanford Univ.; 11/07; (iii) Séminaire Mathématiques Appliquées à la Génomique: Modèles et Algorithmes, Marseille, 01/08; (iv ) Université de Nice, séminaire du Dpt de Mathématiques, 01/08.
- Colloquium *Les avancées françaises en sciences de l'information présentées par leurs auteurs*, French Academy of Sciences; 2007.
- *Modèles pour la description de la structure des protéines: de la géométrie à la bio-physique en passant par les statistiques*; Bioinformatique, modélisation des systèmes biologiques Journées 2007, ACI-IMPBIO & GDR BIM; 10/07.
- *Geometric and topological inference in the non linear realm: on the importance of singularity theory*; Non-Linear Computational Geometry, Institute for Mathematics and its Applications, Univ. of Minnesota; 06/07.
- *Geometry and topology for structural molecular modeling: erroneous judgments and (moderately) high hopes*; Bioinformatics: algorithms, structures and statistics, Workshop of the LIX, Ecole Polytechnique, France; 12/05.
- *Modeling interfaces of macro-molecular complexes*; Visualization of Large Biomolecular Complexes Workshop, La Jolla; 09/05.

## 14 Scientific responsibilities

### 14.1 Program committees

– Applied Geometry, Computer Graphics, Geometry Processing:

- Symposium on Computational Geometry: 2019
- Symposium On Geometry Processing: 2003, 2004, 2005, 2006, 2007, 2008, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019
- Shape Modeling International: 2016
- Geometric Modeling and processing: 2012

- Computer Graphics International: 2013
  - SIAM Conference on Geometric and Physical Modeling: 2011
  - ACM Symposium on Solid and Physical Modeling: 2005, 2006, 2007, 2008, 2012
  - Symposium on Solid and Physical Modeling: 2016, 2017, 2018, 2020
  - Symposium On Point Based Graphics: 2004, 2005, 2006, 2008
  - New Advances in Shape Analysis and GEometric Modeling: 2007
  - International Symposium on 3D Data Processing, Visualization, and Transmission: 2008
- Computational Biology and Computational Structural Biology:
- International Conference on Computational Systems-Biology and Bioinformatics: 2019
  - Intelligent Systems for Molecular Biology (ISMB), PC member of Protein Interactions & Molecular Networks: 2016, 2017, 2018, 2019, 2020.
  - ACM Conference on Bioinformatics, Computational Biology and Biomedical Informatics (ACM BCB): 2013, 2014, 2017
  - IEEE International Conference on BioInformatics and BioEngineering: 2018
  - IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology: 2012
  - International Conference on Pattern Recognition in Bioinformatics: 2008, 2009, 2010, 2011, 2012, 2013, 2016
  - Computational Intelligence Methods for Bioinformatics and Biostatistics: 2013
  - JOBIM: 2017

## 14.2 PhD Thesis and habilitation committees

- Maria Elisa Ruiz Echartea, Université de Lorraine, December 2019. Rapporteur on the PhD thesis *Multi-component protein assembly using distance constraints*. Advisors: David W. Ritchie - Marie-Dominique Devignes.
- Alba Chiara De Vitis, Université Côte d’Azur, May 2019. Committee member. *Kernel Methods for High Dimensional Data Analysis*. Advisors: D. Cohen-Steiner, J-D. Boissonnat.
- Juraj Michalik, Ecole Polytechnique, March 2019. Rapporteur on the PhD thesis *Non-redundant sampling in RNA bioinformatics*. Advisors: Yann Ponty and H el ene Touzet.
- Hugo Schweke, Paris-Saclay University, December 2018. Rapporteur on the PhD thesis *D veloppement d’une m thode in silico pour caract riser le potentiel d’interaction des surfaces prot iques dans un environnement encombr *. Advisors: Marie-H el ene Mucchielli-Giorgi and Anne Lopes.
- Julien Ogor, ENSTA Bretagne, May 2018. Rapporteur on the PhD thesis *Design of algorithms for the automatic characterization of marine dune morphology and dynamics*. Advisor: B. Zerr.
- Rodrigo Dorantes-Gilardi, University of Lyon, April 2018. Rapporteur on the PhD thesis *Bio-Mathematical aspects of the plasticity of proteins*. Advisors: L. Vuillon and C. Lesieur.
- Cl ment Viricel, University of Toulouse, December 2017. Rapporteur on the PhD thesis *Contributions au d veloppement d’outils computationnels de design de prot ines : m thodes et algorithmes de comptage avec garantie*. Advisors: T. Schiex and S. Barbe.
- Huaxiong Ding, University of Lyon, December 2016. Committee member. *Combining 2D facial Texture and 3D face morphology for estimating people soft biometrics: gender, facial expression* Advisors: Liming Chen and Jean-Marie Morvan.
- Mathilde Le Boudic-Jamin, University of Rennes 1, December 2015. Rapporteur on the PhD thesis *Similarit s et divergences, globales et locales, entre structures prot iques*. Advisor: R. Andonov.
- Nathan Desdouits, University Pierre et Marie Curie / Institut Pasteur Paris, May 2015. Rapporteur on the PhD thesis *Concepts et m thodes d’analyse num rique de la dynamique desavit s au sein des prot ines applications   l’ laboration de strat gies novatrices d’inhibition*. Advisors: Michael Nilges and Arnaud Blondel.



- Petr Popov, University of Grenoble, January 2015. Committee member. *New methods for the prediction of protein - protein interactions at the structural level*. Advisor: Sergei Grudinin.
- Didier Devaurs, University of Toulouse, October 2014. Rapporteur on the PhD thesis *Extensions of Sampling-based Approaches to Path Planning in Complex Cost Spaces: Applications to Robotics and Structural Biology*. Advisor: Juan Cortés.
- Juan Cortés, University of Toulouse, April 2014. Rapporteur on the Habilitation thesis *Algorithmics of motion: from robotics, through structural biology, towards atomic-scale CAD*.
- Dave Ritchie, University of Nancy, April 2011. Rapporteur on the Habilitation thesis *High performance algorithms for molecular shape recognition*.
- Duc Thanh Le, University of Toulouse, October 2010. Rapporteur on the PhD thesis *(Dis)assembly path planning for complex objects and applications to structural biology*. Advisors: T. Siméon and J. Cortés.
- Noel Malod-Dognin, University of Rennes, January 2010. Rapporteur on the PhD thesis *Protein structure comparison : From Contact Map Overlap Maximisation to Distance-Based Alignment Search Tool*. Advisor: R. Andonov.
- Mathias Carlen, EPFL, January 2010. Rapporteur on the PhD thesis *Computation and Visualization of Ideal Knot Shapes*. Advisor: J. Maddocks.
- Benjamin Schwarz, University of Strasbourg, September 2009. Rapporteur on the PhD thesis *Application de la théorie des formes- $\alpha$  pour la caractérisation de la surface et des poches de macromolécules biologiques*. Advisor: J-M. Wurtz.
- Adrien Saladin, University of Paris VII, May 2009. Rapporteur on the PhD thesis *Macromolecular docking. Applications to RecA filament*. Advisors: Chantal Prévost and Marting Zacharias.
- Christine Martin, University of Orsay, December 2008. Rapporteur on the PhD thesis *Sélection immersive et guidée par des motifs géométriques spécifiques de sites d'intérêt pour l'amarrage protéine - protéine*. Advisor: A. Cornuéjols.
- Julie Bernauer, University of Orsay, April 2006. Rapporteur on the PhD thesis *Utilisation de la tessellation de Voronoi pour l'étude des complexes protéine-protéine*. Advisors: J. Janin, A. Poupon.
- Cédric Chappuis, UTC Compiègne, 2003. Examiner on the PhD thesis *Optimisation inverse de maillages surfaciques de pièces mécaniques par interpolation diffuse*. Advisor: A. Rassineux.

## 15 Services

### 15.1 Expertise - consulting

- 2017-2019. President of the *Comité de suivi doctoral*, Inria Sophia Antipolis.
- 2010-... Member of the steering committee of the *GDR Bioinformatique Moléculaire*, for the *Structure and macro-molecular interactions* theme.
- 2017-... Co-chair, with Yann Ponty, of the working group / groupe de travail (*GT MASIM - Méthodes Algorithmiques pour les Structures et Interactions Macromoléculaires*, within the *GDR de Bioinformatique Moléculaire* (GDR BIM, <http://www.gdr-bim.cnrs.fr/>).
- 2012. Rapporteur for the European Science Foundation, for the conference on Energy Landscapes ( <http://www.esf.org/conferences/12382> ).
- 2004-07. Member of the Inria *Comité d'Orientation Scientifique et Technologique, Actions Incitatives*, COST-AI —the Inria Scientific Steering Committee.
- 2001–06. Member of the *commission of specialists*, section 25/26 —Mathematics. Steering committee of the Mathematics Dpt of the Bourgogne University, France.
- 2020. Jury of the *Institut Universitaire de France*, section 27.
- 2019. Remote evaluator for *ERC Consolidator Grants*.
- 2016. Expert for the *Italian Research and University Evaluation Agency (ANVUR)*.

- 2013. *European Commission* Panel expert for the 7th Framework Programme 7, Information and Communication Technologies / Future and Emerging Technologies (FET Open).
- 2004,2011. Evaluator for the Austrian Science Foundation —discipline: Applied Geometry.
- 2011-12. Member of the scientific committee of the exposition *Leonard de Vinci: la Nature et l'Invention*, Cité des Sciences, Paris.

## 15.2 Review duties

**Journals, CS.** ACM Transactions on Graphics, SIAM Journal on Computing, Computational Geometry Theory and Applications, IEEE Transactions on Robotics and Automation, IEEE Pattern Analysis and Machine Intelligence, Algorithmica, J. Algorithms, J. of Computational Geometry, Medical Image Analysis, Foundations of Computational Mathematics.

**Journals, Computational (Structural) Biology.** ACM/IEEE Transactions on Computational Biology and Bioinformatics, BMC Systems Biology. BMC Bioinformatics, Journal of Computational Chemistry, Journal of Mathematical Biology, Journal of immunology, Nucleic Acids Researc., Neurocomputing, PLOS Computational biology, Proteins: Structure, Function, Bioinformatics.

**Conferences, CS.** ACM Symposiun on Computational Geometry, ACM Symposiun on Solid Modeling, Eurographics, Symp. Theoretical Aspects of Comp. Sc., Graphics Interface, Computer Graphics Forum, IEEE Visualization, Symp. on Geom. Processing, Symp. on Point Based Graphics, Siggraph, European Symp. on Algorithms, Computer Graphics International.

**Conferences, Computational Biology.** International Conference on Pattern Recognition in Bioinformatics.

# 16 Funding

## 16.1 Applied geometry

2010-13. EU ICT FET open project: *Computational Geometric Learning*, in collaboration with jJena Univ. (coordinator: J. Giesen), Inria (Geometrica Sophia, Geometrica Saclay, ABS), Tech. Univ. of Dortmund, Tel Aviv Univ., Nat. Univ. of Athens, Univ. of Groningen, ETH Zürich, Freie Univ. Berlin.

2010-12. ANR *Geometric Inference and Geometric Approximation*. Coordinator: F. Chazal, Inria Geometrica - Saclay.

2006-09. ACI Jeunes Chercheurs *Geometry Toplogy Algorithms*. With F. Chazal (Univ. Dijon), D. Attali (CNRS Grenoble), M. Pocchiola (ENS Ulm).

2005-07. FET Open project *Algorithms for Complex Shapes with certified topology and numerics*, FP6 IST-006413. Project involving Univ. Groningen, ETH Zurich, Freie Univ. Berlin, Inria, MPI Saarebrucken, Univ. Athens, Tel Aviv Univ., Geometry Factory.

2001-04. FET Open European project *Effective Computational Geometry for Curves and Surfaces*. Project involving Univ. Groningen, ETH Zurich, Freie Univ. Berlin, Inria, MPI Saarebrucken, Tel Aviv Univ.

1998-2000. Program *Factory for the future*, funded by AFIRST (Association Franco-Israélienne pour la recherche scientifique et technologique). With D. Halperin and M. Sharir (Tel Aviv Univ.).

## 16.2 Molecular modeling

2012-13. PEPS CNRS/INSERM/Inria. *Novel approaches to characterizing energy landscapes for flexible macromolecular systems in biology*. With C. Robert, from Inst. Biologie Physico-chimique/CNRS, Paris.

2012-13. PEPS CNRS/INSERM/Inria. *Modeling Large Protein Assemblies with Toleranced Models*. With V. Doye, from Inst. Jacques Monod, Paris.

2007-08. France-Stanford center for Interdisciplinary Studies. *Developments of Geometric Methods and Algorithms for the study of macro molecular assemblies*. With M. Levitt, Dpt of Structural Biology, Stanford Univ.

2006-07. Inria Collaborative Research Action. *Revisiting the Flexibility of Proteins*. With M. Nilges (Inst. Pasteur, Paris), and J. Giesen (ETH Zurich).

2003-04. Inria Collaborative Research Action, *Protein-Protein Docking*. With B. Maigret (CNRS Nancy) and X. Cavin (Inria Nancy).

1999-2000. Research contract with Elf-Sanofi-Synthélabo —P.I. The contract was geared towards the development of novel algorithms to report and draw similar molecules —for the drug industry.

## 17 Software

### 17.1 The Structural Bioinformatics Library

**The Structural Bioinformatics Library (2008–**. I am the designer and the co-developer, with my former PhD student Tom Dreyfus (now at Google) of the Structural Bioinformatics Library, see <https://sbl.inria.fr/> [17]. The SBL is a generic C++/python cross-platform software library targeting complex problems in structural bioinformatics. Its tenet is based on a modular design offering the following software components:

- (For end-users) Applications solving specific problems in computational structural biology, without compromising robustness and performances.
- (For developers) Broad C++ toolbox with modular design, involving core algorithms, biophysical models, and modules.
- (For students) Jupyter notebooks combining snippets of code and illustrations of results.

With circa 80 C++ packages, 400,000 of C++ code, more than 1000 C++ classes and 1,500 pages of documentation, the SBL represents a major endeavor.

We anticipate that the recently proposed Conda based installation and Jupyter notebooks will expand its user base very significantly, making it a premier software resource in structural bioinformatics.

### 17.2 Software development until 2014

In the sequel, we only list the software which is not part of the Structural Bioinformatics Library.

**2006; Jet\_fitting\_3** C++ CGAL package to estimate the differential properties of a smooth discretized surface. With M. Pouget.  
Integrated to CGAL <http://www.cgal.org>.  
Publications: [31, 32]

**2006; Ridges\_3** C++ CGAL package to estimate the curves of extremal curvature of a smooth discretized surface. With M. Pouget.  
Integrated to CGAL <http://www.cgal.org>.  
Publication: [87]

**2001; Nuages-pc** A C++ program reconstructing surfaces from unorganized point clouds. 20,000 lines of code. Purchased by Dassault Systèmes for the CATIA CAD system after a six month evaluation against the market solutions.  
Integrated to CATIA v-5.  
Publications: [5, 6]

**1997; Module in Combstruct** *Maple* module performing asymptotics of rational fractions with rational coefficients for the *Combstruct* library. Project Algorithms, Inria Rocquencourt.

## 18 Personal interests

- Currently: triathlon, biking (road and mountain biking), mountaineering (rock climbing, mountaineering, randonnee skiing).
- Formerly: soccer, horse riding.