Antonio Mucherino's Curriculum Vitæ

Personal

Antonio Mucherino (born in 1978)
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Job history and experiences

Current position (since Sep 2011):

- **Associate Professor**[1] at IRISA, University of Rennes 1, Rennes, France.

Previous positions:

- **Postdoc Researcher**, *from Sep 2006 to Aug 2011*, in inverse chronological order

time	*where*	*advisor(s)*
9 months	CERFACS, Toulouse	Serge Gratton, Iain Duff
1 year	INRIA Lille	El-Ghazali Talbi
1.5 years	LIX, École Polytechnique, Palaiseau	Carlile Lavor, Leo Liberti
9 months	IFAS, University of Florida	Petraq Papajorgji
6 months	CAO, University of Florida	Panos Pardalos

- **Junior Researcher** (during PhD), *from Nov 2001 to Dec 2005*

time	*where*	*advisor*
10 months	ISA-CNR, Avellino	Angelo Facchiano
10 months	Giovanni Pascale Foundation, Naples	Giovanni Colonna

- **Trainee** (before PhD)

time	*where*	*advisor*
3 months	ICAR-CNR, Naples	Marco D'Apuzzo

[1] Equivalent in France to *Maître de Conférences* with *Habilitation à Diriger des Recherches*.

Education

- *July 2018*
  Habilitation à Diriger des Recherche (HDR),
  University of Rennes 1, France.
  HDR Monograph title: *On the Discretization of Distance Geometry: Theory, Algorithms and Applications.*
  Awarded on: July 17^{th}, 2018. President of the committee: Kadi Bouatouch.

- *Since 2009*
  On the **Qualification Lists** for "Maître de Conférences",
  French National University Council (CNU), Section: 27 (computer science).

- *Nov 2001 - Dec 2005*
  PhD in Computational Biology,
  Department of Mathematics, Second University of Naples, Italy.
  Thesis title: *Geometric Aspects in the Simulation of Protein Folding Processes.*
  Awarded on: December 13^{th}, 2005. Supervisor: Marco D'Apuzzo.

- *Sep 1997 - Oct 2001*
  Master in Mathematical Sciences,
  Department of Mathematics, Second University of Naples, Italy.
  Thesis title: *Quadratic Optimization: Algorithms and Software for Dense Problems.*
  Awarded on: October 30^{th}, 2001. Supervisor: Marco D'Apuzzo.

Research interests

- Distance Geometry
- Data Mining
- Meta-Heuristics
- Bioinformatics
- Parallel Computing

Research activities

Distance Geometry

The Distance Geometry Problem (DGP) asks whether a simple weighted undirected graph $G = (V, E, d)$ can be realized in a K-dimensional space so that the distance between each pair of realized vertices u and $v \in V$ is the same as the weight d_{uv} assigned to the edge $\{u, v\} \in E$, when available [11]. The embedding space is Euclidean in most applications. The distance information can be given either through one real value, representing an exact distance or rather an approximation, or by real-valued intervals. The DGP is NP-hard, and in recent years I have been working on the different facets of this problem with several colleagues, and mostly with Leo Liberti, Carlile Lavor, Douglas Gonçalves and Nelson Maculan. We have published several papers on this topic [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 26, 33, 34, 36, 38, 39, 40, 41, 42, 43, 44, 46, 50, 51, 52, 53, 55, 56, 57, 58, 59, 63, 65, 66, 67, 68, 73, 74, 75, 76, 87, 77, 79, 80, 81, 82, 83, 84, 85, 86, 88, 89, 90, 93, 94, 95, 96, 97].

Different applications can lead to the definition of a DGP: the DGP can nowadays be seen as a classical operational research problem. One classical DGP application arises in biology: experiments of Nuclear Magnetic Resonance (NMR) are able to find estimates of some distances between atom pairs in molecules, which can then

be exploited for discovering molecular conformations [67]. Recently, we also began to investigate the possibility to formulate as a DGP a particular class of the Multidimensional Scaling (MDS) [34]. More recently, we have also started to work on human motion adaptation by a novel distance-based approach, which brings to the definition of a DGP [32, 73]. Since motions have a temporal component, it was necessary to preliminary extend the DGP to dynamical problems [2, 33]. Currently, this is my main research line.

The discretization of the DGP can be performed when some particular assumptions are satisfied. These ensure that every vertex $v \in V$ has at least K adjacent predecessors in G, that can serve as a reference for computing candidate positions for v [16]. Moreover, in order to deal with real-life data, where distances are generally imprecise and often represented by intervals, it is required that at least $K-1$ reference distances can be considered as exact [13]. These assumptions allow for defining the set of possible positions for a given vertex v as the intersection of K Euclidean objects: hyper-spheres, that are related to exact distances, and hyper-spherical shells, that are related to non-exact distances [9]. These intersections give either discrete subsets of positions, or continuous objects in dimension 1. In the latter case, with a little loss of information, we can discretize the obtained continuous object by selecting some sample positions [13]. The discretization allows to define a tree of possible vertex positions, which corresponds to the search domain of the DGP after the discretization. The discretization does not change the problem complexity, which remains NP-hard [16].

Algorithms based on a *branch-and-prune* (BP) framework can be implemented for exploring the search domain of discretizable DGPs [13]. We developed numerically stable methods for the computation of candidate vertex positions [9, 16] at every layer of the search tree. Once computed, the feasibility of candidate positions is verified by employing the so-called pruning devices [8, 40, 51, 82]. Pruning allows to focus the search on the feasible regions of the search tree. Basic pruning is based on the verification of the distances that are not used during the discretization process [16]. These distances actually allow to define additional Euclidean objects to be intersected with the K objects involved in the discretization [39]. Additional pruning devices can be conceived and tailored to some particular class of DGP instances, such as the DGP class related to biological molecules [8, 51]. We also integrated the algorithm with some energy-based pruning devices, where van der Vaals and Lennard Jones potentials are taken into consideration [40]. The enumeration of the entire solution set of DGP instances can be performed by our approach. MD-JEEP is an implementation of a BP algorithm for discretizable DGPs with exact distances [53], that is freely distributed (see section "Developed software" below). In presence of a large number of wrong measurements, it may be necessary to relax the algorithm pruning phase, which implies an increase of the number of nodes included in the search tree: heuristics can in this case be conceived for speeding up the search [59]. The BP framework was recently enhanced for problems in dimension 1, where an additional pruning phase, named *backtracking pruning*, allows to deal with interval distances without introducing any approximations on the distances [63]. Current research is aimed at extending such a result to dimensions $K > 1$.

At the beginning of our work on the DGP, we have focused our attention on instances where all available distances are exact. This is evidently an unrealistic assumption for many real-life applications, but it allowed us to study some interesting properties of discretizable DGPs. We discovered in fact that the discrete search domain of some DGPs contains several symmetries [50], which can be exploited for computing its solution set [4, 21, 46]. Moreover, when DGP instances related to molecular conformations are considered, the search domain is a tree with bounded width, so that it can never experience a combinatorial explosion [79]. The particular structure of this tree also allowed us to develop two parallelization strategies for the BP framework [44, 55], which were tested on the French nation-wide grid infrastructure Grid5000 (`www.grid5000.fr`).

A *discretization order* is a vertex order for the graph G such that the discretization assumptions are satisfied [7, 10, 13, 17, 19, 26, 36, 38, 41, 42, 52, 58, 65, 75, 76, 84, 86]. For an automatic detection of discretization orders, a greedy algorithm was proposed in [17] and extended subsequently for dealing with interval distances in [41]. In both cases, it was proved that the greedy algorithm is able to identify discretization orders, when they exist, and to deliver a certificate of non-existence otherwise. An ad-hoc heuristic, that has as worst-case complexity the one of the greedy algorithm, was also proposed in [76] in order to deal with very large instances. The complexity of this ordering problem can become NP-hard when additional requirements are integrated with the discretization assumptions. For example, the "consecutivity assumption" requires that all reference vertices for a given vertex $v \in V$ are consecutive in the order, and that they immediately precede v. When this additional assumption is satisfied, all reference distances are edges of cliques belonging to G, and the discretization order

can be defined as a sequence of overlapping cliques [38]. A pseudo de Bruijn graph was developed in [38] for aiding the task of generating discretization orders satisfying the consecutivity assumption, and an ordering for the protein backbones that is optimal in terms of length was found. Other orders satisfying the consecutivity assumption were previously handcrafted for the protein backbone [13] and the side chains belonging to the amino acids involved in the protein synthesis [10].

We also worked on suitable methods for finding discretization orders satisfying a given set of objectives, together with the necessary discretization assumptions [7, 36, 65, 83, 84, 86]. In [65], we developed a constraint program to this purpose, and we found an optimal (partial) discretization order for the protein backbones by solving this program by Answer Set Programming (ASP). In [36], this problem is instead tackled from a theoretical point of view, while we proposed an algorithm (having polynomial complexity) for the generation of optimal discretization orders in [7], where the objectives to be optimized are given by a set of simple functions.

The theory and the algorithms developed for discretizable DGPs can be potentially extended to other well-known problems. Protein folding refers to the body of knowledge related to the study of protein conformations by exploiting only their chemical composition. Work performed during my PhD showed that geometry can play an important role in the identification of protein folds [22, 71, 99]. We also investigated the possibility of discretizing the set of feasible protein folds for a given molecular chemical composition [77]. Also interesting is to verify whether ideas, initially developed for the protein folding, can be exploited for solving other problems related to protein molecules [40]. This will be the topic of future research.

Data mining

Data mining consists in extracting previously unknown, potentially useful and reliable patterns from a given set of data. During my postdoc at University of Florida, in collaboration with Panos Pardalos and Petraq Papajorgji, I wrote a textbook describing the most common data mining techniques [27]. The book also contains many applications of data mining to the agricultural field, as well as to some related fields, such as biology and chemistry. Surveys on the same topic can be found also in [23] and [49].

In recent years, in collaboration with Leo Liberti, I have been working on supervised biclustering techniques for classification. Given a set of data, biclustering aims at finding simultaneous partitions in biclusters of its samples and of the features which are used for representing the samples. Consistent biclusterings can be exploited for performing supervised classifications, as well as for solving feature selection problems. The problem of identifying a consistent biclustering can be formulated as a 0–1 linear fractional optimization problem, which is NP-hard. We are working on a bilevel reformulation of this optimization problem, and on a heuristic which is based on the bilevel reformulation (see section "Meta-Heuristics" below). In [47], I extended this technique to sets of data containing negative entries.

As pointed out in our book [27], biclustering had never been applied to agricultural problems before the book publication, while the application seemed to be in fact promising. Subsequently, we applied biclustering to the analysis of wine fermentations [48, 54]. The problem consists in predicting problematic fermentations at the early stages of the process: we discovered some compounds of wine that may be the cause of problematic fermentations [54]. This is a joint work with Alejandra Urtubia.

Meta-Heuristics

Meta-heuristics are widely employed in optimization. My first experience with meta-heuristics dates back to my PhD in Italy, where I was working on a geometric model for the simulation of protein conformations [101]. This model leads to the definition of a global optimization problem, whose solutions represent geometrically well-shaped conformations for proteins, that we were used to obtain by executing a simple Simulated Annealing (SA). The permutations implemented in our SA implementations were particularly inspired by the geometric nature of the considered problem [24, 71, 99].

A few years later, I took part of the development of a novel meta-heuristic framework which is inspired by the behavior of a monkey climbing trees of solutions with the aim of finding good-quality solution approximations [61, 62, 70]. We named this method Monkey Search (MS). Rather than a completely new meta-heuristic approach,

MS can be seen as a general framework (describing the monkey behavior) where other ideas and strategies for global optimization can be implemented. This work was performed in collaboration with Onur Seref, during my postdoc at University of Florida.

In the context of data mining, we have been working on techniques for supervised biclustering (see section "Data Mining" above). We proposed a bilevel reformulation of the associated optimization problem, where the inner problem is linear, and its solutions are also solutions to the original problem [69, 92, 98]. In order to solve the bilevel problem, we have developed an algorithm that performs a Variable Neighborhood Search (VNS) in the space defined by the outer problem, while the inner problem is solved exactly by CPLEX at each VNS iteration (see section "Developed software" below).

More recently, Stefka Fidanova, Maria Ganzha and myself proposed the *environment* as a general concept in meta-heuristics [37, 64]. As of today, we have tested this novel idea in conjunction with only one meta-heuristic: the Ant Colony Optimization (ACO). In ACO, artificial ants move in a mathematical space by following the pheromone trails left by ants having previously explored the same region of the search space. Our environment perturbs the perception of the pheromone, for ants to avoid to get trapped at local optima of the considered problem. In a recent work, we used our ACO with environmental changes for inter-criteria analysis [35]. Work is in progress for a theoretical study for this new meta-heuristic concept, as well as for testing this novel idea with other meta-heuristic frameworks.

Teaching

Only information about the classes I am currently teaching are reported below.
More details about all courses I have given, as well as some didactic material, can be found at the address: `http://www.antoniomucherino.it/en/teaching.html`

1. **Multithreading Operating Systems** (in English).
   `eit Digital` Master School, Master in Informatics, University of Rennes 1.
   Academic year 2018/19, first semester, level M1 (M.Sc).
2. **Parallel Computing** (in English).
   `eit Digital` Master School, University of Rennes 1.
   Academic year 2018/19, second semester, level M1 (M.Sc).
3. **An Introduction to Object Oriented Programming** (in French, "Programmation à objets").
   Bachelor of Science in Informatics, University of Rennes 1.
   Academic year 2018/19, first semester, level L2 (B.Sc).
4. **An Introduction to Programming with Java** (in French, "Informatique 1").
   Bachelor of Science in Informatics, University of Rennes 1.
   Academic year 2018/19, first semester, level L1 (B.Sc).

In March 2018, I gave a lecture on *distance geometry and applications* to a group of Master students of the Department of Mathematics of UFSC (Florianópolis, Santa Catarina, Brazil).

Previous courses were given at University of Rennes 1 (since academic year 2011-12), at the École Polytechnique in Palaiseau (France) and at the Second University of Naples (Italy).

Projects

Awarded Grants

1. *Rapid NMR Protein Structure Determination and Conformational Transition Sampling by a Novel Geometrical Approach*. International cooperation between IRISA and Academia Sinica (Taipei, Taiwan). Source:

CNRS-MoST, 5kEUR per year, 2018–19.

2. *The Special Role of Topology in the Analysis and the Simulation of Human Behaviors.* Temporary part-time job as an INRIA researcher (délégation INRIA). Source: INRIA Rennes, 8kEUR per year, 2016–2017.

3. *On the Generalization of the Distance Geometry and its Applications.* Interdisciplinary research. Source: INS2I/CNRS, 7kEUR, 2016.

4. *Distance Geometry and Applications.* International cooperation between University of Rennes 1 and Brazilian partners. Source: University of Rennes 1, 2kEUR per year. Awarded every year from 2012 to 2016.

5. *Distance Geometry and Answer Set Programming.* 1-year postdoc at University of Rennes 1. Source: Brittany Region, 33kEUR (75% of total cost), 2013.

6. *Discretizable Molecular Distance Geometry Problem and Protein Docking Problem.* 2-month visit (*chaire*) to UNICAMP (São Paulo, Brazil) for myself. Source: UNICAMP and French Embassy in São Paulo, travel and stay, 2012.

7. *Wine Fermentation Analysis by Biclustering.* International cooperation between IRISA and the Universidad Técnica Federico Santa Maria, Valparaíso, Chile. Source: CNRS-CONICYT, 4kEUR, 2012.

8. *A Discrete Approach to the Molecular Docking Problem.* 1-month visit to University of Rennes 1 for C. Lavor. Source: ISTIC, University of Rennes 1, 3kEUR, 2012.

Participation

9. *Modelling Human Motion for Synthesis and Recognition with Deep Learning on Surface Features.* Royal Society International Exchanges. Source: UK's Royal Society, 12kGBP, 2019-20.

10. *An Interval Branch-and-Prune Approach for Obtaining Intrinsically Disordered Protein Conformations*, "Infinity" interdisciplinary projects, CNRS, 2018.

11. *Geometria de distâncias aplicada ao Cálculo de Estruturas 3D de Proteínas*, UNIVERSAL CNPq project, 2014.

12. *Bayesian inference paradigm: Biology in processors* (Bip:Bip), ANR project, 2012–2017.

13. *Combinatorial Methods to Calculate Protein Structures by Using NMR Data*, State of São Paulo Research Foundation - FAPESP, 2009–2011.

14. *Innovative Problems and Methods in Nonlinear Optimization*, PRIN Project, Italian Ministry of University and Research (MIUR), 2005–2007.

15. *Computational Procedures for Simulating Protein Folding Processes*, Italian Region *Campania* (L.R. n.5 28/3/2002), 2005–2006.

Organization activities

Organization of Scientific Events

- chair of
  - Distance Geometry Day (DGD16), at IRISA/INRIA Rennes, on December 7^{th}, 2016.
    `http://www.antoniomucherino.it/events/DGD16/`

Invitation-based scientific program.

- co-chair of
  - DIMACS Workshop on Optimization in Distance Geometry, at DIMACS Center, Rutgers University (USA), on July 2019.

    `http://dimacs.rutgers.edu/events/details?eID=322`

    Precise dates and scientific program to be announced. Co-chairing with N. Krislock and C. Lavor.

  - Workshop on Computational Optimization (WCO*), in the framework of the Federated Conference on Computer Science and Information Systems (FedCSIS).

    `https://fedcsis.org/wco`

    Co-chairing with D. Zaharie and S. Fidanova since 2012 edition. Workshop held every year in September.

- international advisory committee member for
  - International Conference on Algebra, Number Theory and Discrete Geometry (dedicated to the 80^{th} anniversary of M. Deza birth), TSPU of Leo Tolstoy, Tula, Russia, May 2019.
  - International Conference on BioInformatics and BioEngineering (BIBE18), Taichung, Taiwan, October 2018.
  - Geometric Science of Information (GSI17), Paris, France, November 2017.
  - Many Faces of Distances (MFD14), Campinas, São Paulo, Brazil, October 2014.
  - Distance Geometry and Applications (DGA13), Manaus, Amazonas, Brazil, June 2013.
  - Data Mining in Agriculture (DMA*), editions 2011, 2012 and 2013, in the framework of the "Industrial Conference on Data Mining" (ICDM*).
- session organizer in
  - GSI17, Paris, France, November 7–9, 2017 (with D. Gonçalves).
  - IFORS14, Barcelona, Spain, July 13–18, 2014 (with N. Maculan).
  - ICCOPT13, Lisbon, Portugal, July 27 – August 1, 2013 (with C. Lavor).
  - ISMP12, Berlin, Germany, August 19–24, 2012 (with N. Maculan).
- local organizing committee member for
  - TOGO10, Toulouse, France, August 31 – September 3, 2010.
  - CTW09, Paris, France, June 2–4, 2009.
- local events
  - MimeTIC's Classification Days (CDs), four editions between 2016 and 2017.

    `http://www.antoniomucherino.it/events/CDs/`

Reviewing tasks

- refereed papers for:
  - JOGO, OPTL, JOTA, JOCO, COAP, MATR A and B, ORIJ, ANOR, NCAA, PLSO, IJEPES, SpringerPlus (Springer);
  - DAM, INS, CAM, CAMWA, PRLetters, COMPAG, JBIOTEC, CBAC (Elsevier);
  - GOMS (Taylor & Francis);
  - ITOR, MMA (Wiley);
  - IJNS (World Scientific);
  - IJMHEUR (Inderscience);
  - OJDM (Scientific Research, an Academic Publisher);
  - Biology, Symmetry, Sensors (MDPI);
  - Fundamenta Informaticae, Integrated Computer-Aided Engineering (IOS Press).
- reviewer for Springer books;
- reviewer of projects for INRIA team international partnerships.

International Relationships

- Responsible of the international relationships at ISTIC, University of Rennes 1.
  Since January 2014, I'm member of the *Commission Affaires Internationales* (CAI) at University of Rennes 1.
  The following agreements were recently signed:
  - University of Vienna, Austria (Erasmus+)
  - University of Trento, Italy (Erasmus+)

Conferences and Workshops with contribution

Only conference and workshop acronyms and a few more details are provided in the following list.
More information can be found at: `http://www.antoniomucherino.it/en/conferences.html`

1. WCO18, FedCSIS18, Poznan, Poland. September 9–12, 2018.
2. NMR_Theory_and_Methods, Campinas, São Paulo, Brazil. May 21–22, 2018. [**invited speaker**]
3. GOR-DG17, Bad Honnef, Germany. November 23–24, 2018. [**invited speaker**]
4. MIG17, Barcelona, Spain. November 8–10, 2017.
5. GSI17, Paris, France. November 7–9, 2017.
6. IGRV17, Rennes, France. October 23–27, 2017.
7. WCO17, FedCSIS17, Prague, Czech Republic, September 3–6, 2017.
8. ROADEF17, Metz, France. February 22–24, 2017.
9. WCO16, FedCSIS16, Gdansk, Poland. September 11–14, 2016.
10. AIMSA16, Varna, Bulgaria. September 7–9, 2016.
11. WCO15, FedCSIS15, Lodz, Poland. September 13–16, 2015.
12. LSSC15, Sozopol, Bulgaria. June 8–12, 2015.

13. IWBBIO15, Grananda, Spain. April 15–17, 2015.
14. ROADEF15, Marseille, France. February 25–27, 2015.
15. MFD14, Campinas, São Paulo, Brazil. October 22–24, 2014 (*two contributions*).
16. WCO14, FedCSIS14, Warsaw, Poland. September 7–10, 2014.
17. IFORS14, Barcelona, Spain. July 13–18, 2014.
18. Uncertainties14, Rouen, France. June 23–27, 2014.
19. INFORMS13, Minneapolis, USA. October 6–9, 2013 (*two contributions*).
20. WCO13, FedCSIS13, Krakov, Poland. September 8–11, 2013.
21. GSI13, Paris, France. August 28–30, 2013.
22. ICCOPT13, Lisbon, Portugal. June 27 – August 1, 2013.
23. DGA13, Manaus, Amazonas, Brazil. June 24–27, 2013. [**invited speaker**]
24. IWBBIO13, Granada, Spain. March 18–20, 2013.
25. Computational Biomedicine, Gainesville, Florida, USA. January 24–26, 2013.
26. Ottawa Symposium on Biochemistry & Biophysics, Ottawa, USA. October 24–25, 2012.
27. INFORMS12, Phoenix, USA. October 14–17, 2012.
28. CLAIO12, Rio de Janeiro, Brazil, September 24–28, 2012.
29. WCO12, FedCSIS12, Wroclaw, Poland, September 9–12, 2012.
30. ISMP12, Berlin, Germany, August 19–24, 2012 (*two contributions*).
31. ICMRBS12, Lyon, France, August 19–24, 2012.
32. 2012 SIAM Annual Meeting, Minneapolis, Minnesota, USA, July 9–13, 2012.
33. MDA12, Varna, Bulgaria, July 2–5, 2012.
34. GOW12, Natal, Brazil, June 26–29, 2012.
35. PCO12, IPDPS12, Shanghai, China, May 21–25, 2012.
36. ROADEF12, Angers, France, April 11–13, 2012.
37. br.BIO.fr 2012, Paris, France, March 21, 2012.
38. CSBW11, BIBM11, Atlanta, GA, USA, November 12–15, 2011.
39. WCO11, FedCSIS11, Szczecin, Poland, September 18–21, 2011.
40. MAS11, Rome, Italy, September 12–14, 2011.
41. DMA11, ICDM11, New York City, USA, September 2, 2011.
42. COCOA11, Zhangjiajie, China, August 4–6, 2011.
43. IFORS11, Melbourne, Australia, July 10–15, 2011.
44. WCGO11, Crete, Greece, July 3–7, 2011 (*two contributions*).
45. CTW11, Frascati, Rome, June 14–16, 2011 (*two contributions*).
46. LSSC11, Sozopol, Bulgaria, June 6–10, 2011.
47. ISBRA11, Changsha, China, May 27–29, 2011.
48. SEA11, Crete, Greece, May 5–7, 2011.
49. ROADEF11, Saint Etienne, France, March 2–4, 2011.
50. IWCP10, BIBM11, Hong Kong, December 18–21, 2010.

51. META10, Djerba, Tunisia, October 27–31, 2010.
52. ICMS10, Kobe, Japan, September 13–17, 2010.
53. TOGO10, Toulouse, France, August 31 – September 3, 2010.
54. DMA10, ICDM10, Berlin, Germany, July 14, 2010.
55. EURO10, Lisbon, Portugal, July 11–14, 2010.
56. DMBIO10, Crete, Greece, July 7–9, 2010.
57. EU/MEeting 2010, Lorient, France, June 2–4, 2010.
58. AICCSA10, Hammamet, Tunisia, May 16–19, 2010.
59. Grid5000 Spring School 2010, Lille, France, April 6–9, 2010.
60. ROADEF10, Toulouse, France, February 24–26, 2010.
61. CSBW09, BIBM09, Washington D.C., USA, November 1–4, 2009.
62. ICBB09, Venice, Italy, October 28–30, 2009.
63. WCO09, IMCSIT09, Mragowo, Poland, October 12–14, 2009.
64. IFIP09, Buenos Aires, Argentina, July 27–31, 2009.
65. GECCO09, Montréal, Canada, July 8–12, 2009.
66. Engineering Systems Symposium at MIT, Cambridge, Massachusetts, USA, June 15–17, 2009.
67. CTW09, Paris, France, June 2–4, 2009.
68. FAME09, Orlando, Florida, USA, May 14–17, 2009.
69. SAC09, Honolulu, Hawaii, USA, March 8–12, 2009.
70. ROADEF09, Nancy, France, February 10–12, 2009.
71. BBCC08, Avellino, Italy, December 12, 2008.
72. Workshop "Journée Optimeo", Université Paris-Sud XI, Orsay, France, November 21, 2008.
73. ARS Workshop, École Polytechnique, Palaiseau, France, October 31, 2008.
74. CCO08, Gainesville, Florida, USA, January 30 – February 1, 2008.
75. Protein Folding Workshop, Minneapolis, USA, January 14–18, 2008.
76. Biomedicine07, Gainesville, Florida, USA, March 28–30, 2007.
77. BBCC06, Avellino, Italy, December 18, 2006.
78. Biomedicine05, Gainesville, Florida, USA, February 2–4, 2005.
79. CMS04, Neuchatel, Switzerland, April 2–5, 2004.
80. Unravelling Nature's Networks, Sheffield, England, July 20–22, 2003.

Visiting Terms and Seminars

My active collaboration with Brazilian colleagues, working at different Universities in Brazil, is great opportunity for me travel to Brazil. This is a summary per year of my visits and given seminars:

2018 12 days at UFSC; 7 days at UNICAMP (NMR workshop);
2017 7 days at UNICAMP;
2016 10 days at UFSC; 14 days at UNICAMP (2 visits);
2015 7 days at UFSC (1 seminar);
2014 5 days at UNICAMP (MFD workshop);
2013 7 days at UFRJ; 7 days at UNICAMP;
2012 2 month *chaire* at UNICAMP (1 seminar);
2011 10 days at UNICAMP; 2 weeks at UFRJ (1 seminar);
2010 2 weeks at UNICAMP (1 seminar);
2009 7 days at UFRJ.

Colleagues and visited Universities:

- COPPE, UFRJ, Rio de Janeiro, Nelson Macular (Professor Emerito);
- IMECC, UNICAMP, Campinas (São Paulo), Carlile Lavor (Full Professor);
- DM, UFSC, Florianópolis (Santa Catarina), Douglas Gonçalves (Assistant Professor).

This is my list of other visiting terms and seminars:

1. Institut Pasteur, Paris, France. 1 seminar (in the framework of our CNRS Infinity project). Invited by T. Malliavin. June 2018.
2. Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan. 2 weeks (in the framework of our joint CNRS-MoST project). Invited by J-H. Lin. June 2018.
3. Department of Control Systems and Mechatronics, Wroclaw University of Science and Technology, 3 days, 1 seminar. Invited by P. Drag. March 2018.
4. IFSTTAR, Paris, France. 1 seminar. Invited by E. Dumont. November 2017.
5. Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan. 10 days, 1 seminar. Invited by J-H. Lin. June 2017.
6. Institute of Computer Technology, TU Vienna, Austria. 3 days, 1 seminar. Invited by N. TaheriNejad. April 2017.
7. Laboratoire d'Informatique, Université d'Avignon, Avignon, France. 3 days, 1 seminar. Invited by R. Figueiredo. November 2016.
8. INSA, Rennes, France. 1 seminar. Invited by M. Haddou. June 2016.
9. Institut für Informatik, Universität Potsdam, Germany. 4 days, 1 seminar. Invited by T. Schaub. April 2016.
10. Universidade de Aveiro, Portugal. 4 days, 1 seminar. Invited by A. Agra. May 2015.
11. BAS, Sofia, Bulgaria. 3 days, 1 seminar. Invited by S. Fidanova. June 2014.
12. ENSTA Bretagne, Brest, France. 1 seminar during the workshop "Set Computational for Control". Invited by J. Ninin. December 2013.
13. Department of Informatics, UNIFI, Florence, Italy. 1 seminar. Invited by F. Schoen. December 2012.
14. Universidad Técnica Federico Santa Maria, Valparaíso, Chile. 2 weeks. Invited by A. Urtubia. CNRS-CONICYT project. November 2012.
15. BIA, INRA, Toulouse, France. 1 seminar. Invited by M. Vignes. March 2012.

16. Universidad Técnica Federico Santa Maria, Valparaíso, Chile. 7 days, 2 seminars.
    Invited by A. Urtubia. July 2011.
17. LIPN, Université Paris 13, Paris, France. 1 seminar. Invited by R.W. Calvo. April 2011.
18. LIRMM, Université Montpellier 2, Montpellier, France. 1 seminar. Invited by O. Gascuel. April 2011.
19. IRIT, Toulouse, France. 1 seminar. Invited by F. Messine. April 2011.
20. LAMIH, Université de Valenciennes, Valenciennes, France. 1 seminar. Invited by S. Hanafi. March 2011.
21. CERFACS, Toulouse, France. 1 seminar. Invited by I. Duff. June 2010.
22. LRI, Université Paris 11, Orsay, France. 1 seminar. Invited by Ch. Froidevaux. April 2010.
23. Département de Mathématiques et d'Informatique, Université de Reims Champagne-Ardenne,
    Reims, France. 1 seminar. Invited by M. Krajecki. April 2010.
24. LIPADE, Université Paris Descartes, Paris, France. 1 seminar. Invited by M. Nadif. April 2010.
25. ENSEEIHT, Toulouse, France. 1 seminar. Invited by P.R. Amestoy. March 2010.
26. IRISA, Rennes, France. 1 seminar. Invited by R. Andonov. December 2009.
27. Université Paris 11, Orsay, France. 1 seminar. Invited by A. Lisser. April 2009.
28. LAMSADE, Université Paris Dauphine, Paris, France. 1 seminar. Invited by A.R. Mahjoub. March 2009.
29. CIRM, Marseille, France. Invited by M. Hirschowitz. March 2009.
30. DIIGA, Università Politecnica delle Marche, Ancona, Italy. 1 seminar.
    Invited by F. Marinelli. February 2009.
31. Department of Industrial Engineering, University of Florida, Gainesville, USA. 1 seminar.
    Invited by P.M. Pardalos. January 2007.
32. IASI-CNR, Rome, Italy. 1 seminar. Invited by M. Sciandrone. September 2003.

Supervisions

Supervision of postdoc students

- Warley Gramacho, from September 2015 to August 2016.
- Douglas Soares Gonçalves, from April 2013 to March 2014.
- Andrea Cassioli, with L. Liberti (École Polytechnique), from October 2012 to December 2013.

Supervision of PhD students

- Virginia Silva Da Costa, with N. Maculan (Federal University of Rio de Janeiro), defended in 2013.
- Warley Gramacho, with C. Lavor (UNICAMP), defended in 2013.

Supervision of visiting PhD students

- Rafael Santos Alves, PhD student from UNICAMP, Campinas, São Paulo, Brazil, 4 months, 2012.
- Maria Cristina De Cola, PhD student from IASI, CNR, Rome, Italy, 3 months, 2012.

Supervision of Master students

- Florestan De Moor, École Normale Supérieure de Rennes, 2019 (with D. Frey).
- Pierre Le Luron, Université de Rennes 1, 2018 (with S. Collange).
- Florian Elain, INSA Rennes, 2017 (with L. Hoyet and R. Kulpa).
- Antonin Bernardin, Université de Limoges, 2017 (with L. Hoyet).
- Thiruvikkiraman Pandurangan, `eit` Digital, University of Rennes 1, 2016.
- Ivaylo Petrov, IRISA Master Research, University of Rennes 1, 2014.
- Giovanni Cicia, Second University of Naples, 2006 (with M. D'Apuzzo).
- Enrico Raimondo, Second University of Naples, 2004 (with M. D'Apuzzo).
- Matilde Muto, Second University of Naples, 2003 (with M. D'Apuzzo).

Supervision of undergraduate students

- Ariane Postel, Université de Rennes 1, 2016.

Committees

- PhD following committee, Othman Toujier, INSA Rennes, Rennes, years 2018-20, (in French, *comité de suivi individuel doctorant*).
- PhD qualification, Julie Laniau, University of Rennes 1, Rennes, France, October 1^{st}, 2015.
- PhD defense, Germano Abud de Rezende, UNICAMP, Campinas, São Paulo, Brazil, August 28^{th}, 2014.
- Master thesis defense, Master BIG, SVE, University of Rennes 1, Rennes, France, June 20^{th}, 2014.
- PhD defense, Virginia Silva Da Costa, UFRJ, Rio de Janeiro, Brazil, February 21^{st}, 2013.
- PhD defense, Rafael Santos Alves, UNICAMP, Campinas, São Paulo, Brazil, February 25^{th}, 2013.

Computer-related skills

- Programming Languages: C, C++, Java, Fortran 77/90, PHP, Matlab, Python.
- Operating Systems: UNIX, Linux, Windows.
- Linear Algebra Packages: BLAS, LAPACK.
- Optimization Systems and Software: CPLEX, AMPL and others, both commercial and free.
- Parallel Computing Packages: OpenMP, MPI, SCALAPACK, CUDA.

Developed software

MD–JEEP

Implementation of: the Branch and Prune algorithm for distance geometry
Programming language: C
Description: This is an implementation of the Branch & Prune (BP) algorithm for solving discretizable Distance Geometry Problems (DGPs) [14, 16]. MD-JEEP is the result of a strong collaboration among myself, Leo Liberti, Carlile Lavor, Douglas Gonçalves, Nelson Maculan, and other people. The details regarding the discretization of the DGP and the BP algorithm can be found in our publications [1, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 17, 18, 19, 20, 21, 26, 33, 34, 36, 38, 39, 40, 41, 42, 43, 44, 46, 50, 51, 52, 55, 56, 57, 58, 59, 63, 65, 66, 67, 68, 73, 74, 75, 76, 87, 77, 79, 80, 81, 82, 83, 84, 85, 86, 88, 89, 90, 93, 94, 95, 96, 97]. MD-JEEP is distributed under the GNU General Public Licence (v.2). Details about the first release of MD-JEEP can be found in [53].
Sources available for download: `http://www.antoniomucherino.it/en/mdjeep.php`.
Current release: 0.2

BiClust

Implementation of: a heuristic for finding consistent biclusterings in data mining
Programming language: AMPL
Description: This is an implementation of the heuristic described in [69, 98] for finding consistent biclusterings of datasets in data mining. Consistent biclusterings can be exploited for performing supervised classifications in data mining, as well as for feature selection [23, 27, 47, 48, 49, 54, 92].

MS

Implementation of: the Meta-Heuristic Monkey Search
Programming language: C
Description: This software tool implements the meta-heuristic Monkey Search for global optimization. It has been applied to different classes of problems: the problem of identifying Lennard Jones and Morse clusters of molecules [62, 70], the simulation of protein conformations [62, 99], the Multidimensional Assignment Problem (MAP) [61], and the Distance Geometry Problem (DGP) [59].

Languages

- Italian: mother tongue.
- English: excellent spoken and written.
- French: good spoken and written.

Publications

International journals

1. S.J.L. Billinge, Ph.M. Duxbury, D.S. Gonçalves, C. Lavor, A. Mucherino, *Recent Results on Assigned and Unassigned Distance Geometry with Applications to Protein Molecules and Nanostructures*, Annals of Operations Research **271**(1), 161–203, 2018.
2. A. Mucherino, J. Omer, L. Hoyet, P. Robuffo Giordano, F. Multon, *An Application-based Characterization of Dynamical Distance Geometry Problems*, to appear in Optimization Letters, 2018.
3. G. Abud, J. Alencar, C. Lavor, L. Liberti, A. Mucherino, *The K-discretization and K-incident Graphs for Discretizable Distance Geometry*, to appear in Optimization Letters, 2018.
4. F. Fidalgo, D.S. Gonçalves, C. Lavor, L. Liberti, A. Mucherino, *A Symmetry-based Splitting Strategy for Discretizable Distance Geometry Problems*, Journal of Global Optimization **71**(4), 717–733, 2018.
5. D.S. Gonçalves, A. Mucherino, C. Lavor, L. Liberti, *Recent Advances on the Interval Distance Geometry Problem*, Journal of Global Optimization **69**(3), 525–545, 2017.
6. S.J.L. Billinge, Ph.M. Duxbury, D.S. Gonçalves, C. Lavor, A. Mucherino, *Assigned and Unassigned Distance Geometry: Applications to Biological Molecules and Nanostructures*, Quarterly Journal of Operations Research **14**(4), 337–376, 2016.
7. D.S. Gonçalves, A. Mucherino, *Optimal Partial Discretization Orders for Discretizable Distance Geometry*, International Transactions in Operational Research **23**(5), 947–967, 2016.

8. A. Cassioli, B. Bardiaux, G. Bouvier, A. Mucherino, R. Alves, L. Liberti, M. Nilges, C. Lavor, T.E. Malliavin, *An Algorithm to Enumerate all Possible Protein Conformations verifying a Set of Distance Restraints*, BMC Bioinformatics **16**:23, 15 pages, 2015.

9. D.S. Gonçalves, A. Mucherino, *Discretization Orders and Efficient Computation of Cartesian Coordinates for Distance Geometry*, Optimization Letters **8**(7), 2111–2125, 2014.

10. V. Costa, A. Mucherino, C. Lavor, A. Cassioli, L.M. Carvalho, N. Maculan, *Discretization Orders for Protein Side Chains*, Journal of Global Optimization **60**(2), 333–349, 2014.

11. L. Liberti, C. Lavor, N. Maculan, A. Mucherino, *Euclidean Distance Geometry and Applications*, SIAM Review **56**(1), 3–69, 2014.
Awarded **Best of Computing** by ACM Computing Reviews in 2014.

12. L. Liberti, B. Masson, J. Lee, C. Lavor, A. Mucherino, *On the Number of Realizations of Certain Henneberg Graphs arising in Protein Conformation*, Discrete Applied Mathematics **165**, 213–232, 2014.

13. C. Lavor, L. Liberti, A. Mucherino, *The interval Branch-and-Prune Algorithm for the Discretizable Molecular Distance Geometry Problem with Inexact Distances*, Journal of Global Optimization **56**(3), 855–871, 2013.

14. A. Mucherino, C. Lavor, L. Liberti, *The Discretizable Distance Geometry Problem*, Optimization Letters **6**(8), 1671–1686, 2012.

15. A. Mucherino, C. Lavor, L. Liberti, *Exploiting Symmetry Properties of the Discretizable Molecular Distance Geometry Problem*, Journal of Bioinformatics and Computational Biology **10**(3), 1242009(1–15), 2012.

16. C. Lavor, L. Liberti, N. Maculan, A. Mucherino, *The Discretizable Molecular Distance Geometry Problem*, Computational Optimization and Applications **52**, 115–146, 2012.

17. C. Lavor, J. Lee, A. Lee-St. John, L. Liberti, A. Mucherino, M. Sviridenko, *Discretization Orders for Distance Geometry Problems*, Optimization Letters **6**(4), 783–796, 2012.

18. C. Lavor, L. Liberti, N. Maculan, A. Mucherino, *Recent Advances on the Discretizable Molecular Distance Geometry Problem*, European Journal of Operational Research **219**, 698–706, 2012.

19. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *On the Computation of Protein Backbones by using Artificial Backbones of Hydrogens*, Journal of Global Optimization **50**(2), 329–344, 2011.

20. L. Liberti, C. Lavor, A. Mucherino, N. Maculan, *Molecular Distance Geometry Methods: from Continuous to Discrete*, International Transactions in Operational Research **18**(1), 33–51, 2011.
Awarded **ITOR Top Article** in 2013.

21. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *Discrete Approaches for Solving Molecular Distance Geometry Problems using NMR Data*, International Journal of Computational Biosciences **1**(1), 88–94, 2010.

22. A. Mucherino, A. Masello, *Statistical Analysis on the Globular Shape of Protein Conformations*, JP Journal of Biostatistics **4**(1), 1–12, 2010.

23. A. Mucherino, P.J. Papajorgji, P.M. Pardalos, *A Survey of Data Mining Techniques Applied to Agriculture*, Operational Research: An International Journal **9**(2), 121–140, 2009.

24. A. Mucherino, S. Costantini, D. di Serafino, M. D'Apuzzo, A. Facchiano, G. Colonna, *Towards a Computational Description of the Structure of all-alpha Proteins as Emergent Behaviour of a Complex System*, Computational Biology and Chemistry **32**(4), 233–239, 2008.

25. S. Cafieri, M. D'Apuzzo, M. Marino, A. Mucherino, G. Toraldo, *Interior Point Solver for Large-Scale Quadratic Programming Problems with Bound Constraints*, Journal of Optimization Theory and Applications **129**(1), 55–75, 2006.

National journals

26. A. Mucherino, C. Lavor, L. Liberti, N. Maculan, *On the Definition of Artificial Backbones for the Discretizable Molecular Distance Geometry Problem*, Mathematica Balkanica **23**(3-4), 289–302, 2009.

Authored books

27. A. Mucherino, P.J. Papajorgji, P.M. Pardalos, *Data Mining in Agriculture*, 274 pages, Springer, 2009.

Edited books

28. A. Mucherino, C. Lavor, L. Liberti, N. Maculan (Eds.), *Distance Geometry: Theory, Methods and Applications*, 410 pages, Springer, 2013.

Journal special issues

29. A. Mucherino, R. de Freitas, C. Lavor, *Distance Geometry and Applications*, special issue of Discrete Applied Mathematics **197**, 1–144, 2015.

Books of conference proceedings

30. A. Andrioni, R. de Freitas, C. Lavor, L. Liberti, N. Maculan, A. Mucherino (Eds.), *Proceedings of Distance Geometry and Applications* (DGA13), Manaus, Amazonas, Brazil, 2013.

31. S. Cafieri, A. Mucherino, G. Nannicini, F. Tarissan, L. Liberti (Eds.), *Proceedings of the* 8^{th} *Cologne-Twente Workshop on Graphs and Combinatorial Optimization* (CTW09), Paris, France, 2009.

Conference papers (refereed)

32. A. Bernardin, L. Hoyet, A. Mucherino, D.S. Gonçalves, F. Multon, *Normalized Euclidean Distance Matrices for Human Motion Retargeting*, ACM Conference Proceedings, Motion in Games 2017 (MIG17), Barcelona, Spain, 6 pages, 2017.

33. A. Mucherino, D.S. Gonçalves, *An Approach to Dynamical Distance Geometry*, Lecture Notes in Computer Science **10589**, F. Nielsen, F. Barbaresco (Eds.), Proceedings of Geometric Science of Information (GSI17), Paris, France, 821–829, 2017.

34. W. Gramacho, A. Mucherino, J-H. Lin, C. Lavor, *A New Approach to the Discretization of Multidimensional Scaling*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS16), Workshop on Computational Optimization (WCO16), Gdansk, Poland, 601–609, 2016.

35. S. Fidanova, O. Roeva, A. Mucherino, K. Kapanova, *InterCriteria Analysis of Ant Algorithm with Environment Change for GPS Surveying Problem*, Lecture Notes in Artificial Intelligence **9883**, Proceedings of the 17^{th} International Conference on Artificial Intelligence: Methodology, Systems, Applications (AIMSA16), Varna, Bulgaria, 271–278, 2016.

36. A. Mucherino, *Optimal Discretization Orders for Distance Geometry: a Theoretical Standpoint*, Lecture Notes in Computer Science **9374**, Proceedings of the 10^{th} International Conference on Large-Scale Scientific Computations (LSSC15), Sozopol, Bulgaria, 234–242, 2015.

37. A. Mucherino, S. Fidanova, M. Ganzha, *Ant Colony Optimization with Environment Changes: an Application to GPS Surveying*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS15), Workshop on Computational Optimization (WCO15), Lodz, Poland, 495–500, 2015.

38. A. Mucherino, *A Pseudo de Bruijn Graph Representation for Discretization Orders for Distance Geometry*, Lecture Notes in Computer Science **9043**, Lecture Notes in Bioinformatics series, F. Ortuño, I. Rojas (Eds.), Proceedings of the 3^{rd} International Work-Conference on Bioinformatics and Biomedical Engineering (IWBBIO15), Part I, Granada, Spain, 514–523, 2015.

39. D.S. Gonçalves, A. Mucherino, C. Lavor, *An Adaptive Branching Scheme for the Branch & Prune Algorithm applied to Distance Geometry*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS14), Workshop on Computational Optimization (WCO14), Warsaw, Poland, 463–469, 2014.

40. D.S. Gonçalves, A. Mucherino, C. Lavor, *Energy-based Pruning Devices for the BP Algorithm for Distance Geometry*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS13), Workshop on Computational Optimization (WCO13), Krakov, Poland, 335–340, 2013.

41. A. Mucherino, *On the Identification of Discretization Orders for Distance Geometry with Intervals*, Lecture Notes in Computer Science **8085**, F. Nielsen and F. Barbaresco (Eds.), Proceedings of Geometric Science of Information (GSI13), Paris, France, 231–238, 2013.

42. V. Costa, A. Mucherino, C. Lavor, L.M. Carvalho, N. Maculan, *On Suitable Orders for Discretizing Molecular Distance Geometry Problems related to Protein Side Chains*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS12), Workshop on Computational Optimization (WCO12), Wroclaw, Poland, 397–402, 2012.

43. A. Mucherino, C. Lavor, L. Liberti, N. Maculan, *On the Discretization of Distance Geometry Problems*, ITHEA Conference Proceedings, Mathematics of Distances and Applications 2012 (MDA12), Varna, Bulgaria, 160–168, 2012.

44. W. Gramacho, A. Mucherino, C. Lavor, N. Maculan, *A Parallel BP Algorithm for the Discretizable Distance Geometry Problem*, IEEE Conference Proceedings, Workshop on Parallel Computing and Optimization (PCO12), 26^{th} IEEE International Parallel & Distributed Processing Symposium (IPDPS12), Shanghai, China, 1756–1762, 2012.

45. A. Mucherino, M. Fuchs, X. Vasseur, S. Gratton, *Variable Neighborhood Search for Robust Optimization and Applications to Aerodynamics*, Lecture Notes in Computer Science **7116**, I. Lirkov, S. Margenov, J. Wańśiewski (Eds.), Proceedings of the 8^{th} International Conference on Large-Scale Scientific Computations (LSSC11), Sozopol, Bulgaria, 230–237, 2012.

46. A. Mucherino, C. Lavor, L. Liberti, *A Symmetry-Driven BP Algorithm for the Discretizable Molecular Distance Geometry Problem*, IEEE Conference Proceedings, Computational Structural Bioinformatics Workshop (CSBW11), International Conference on Bioinformatics & Biomedicine (BIBM11), Atlanta, GA, USA, 390–395, 2011.

47. A. Mucherino, *Extending the Definition of β-Consistent Biclustering for Feature Selection*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS11), Workshop on Computational Optimization (WCO11), Szczecin, Poland, 269–274, 2011.

48. A. Mucherino, A. Urtubia, *Feature Selection for Datasets of Wine Fermentations*, Proceedings of the 10^{th} International Conference on Modeling and Applied Simulation (MAS11), Rome, Italy, 309–313, 2011.

49. A. Mucherino, G. Ruß, *Recent Developments in Data Mining and Agriculture*, IbaI Conference Proceedings, Proceedings of the Industrial Conference on Data Mining (ICDM11), Workshop on Data Mining in Agriculture (DMA11), New York City, USA, 90–98, 2011.

50. L. Liberti, B. Masson, J. Lee, C. Lavor, A. Mucherino, *On the Number of Solutions of the Discretizable Molecular Distance Geometry Problem*, Lecture Notes in Computer Science **6831**, W. Wang, X. Zhu, D-Z. Du (Eds.), Proceedings of the 5^{th} Annual International Conference on Combinatorial Optimization and Applications (COCOA11), Zhangjiajie, China, 322–342, 2011.

51. A. Mucherino, C. Lavor, T. Malliavin, L. Liberti, M. Nilges, N. Maculan, *Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems*, Lecture Notes in Computer Science **6630**, P.M. Pardalos, S. Rebennack (Eds.), Proceedings of the 10^{th} International Symposium on Experimental Algorithms (SEA11), Crete, Greece, 206–217, 2011.

52. C. Lavor, L. Liberti, A. Mucherino, *On the Solution of Molecular Distance Geometry Problems with Interval Data*, IEEE Conference Proceedings, International Workshop on Computational Proteomics (IWCP10), International Conference on Bioinformatics & Biomedicine (BIBM10), Hong Kong, 77–82, 2010.

53. A. Mucherino, L. Liberti, C. Lavor, `MD-jeep`*: an Implementation of a Branch & Prune Algorithm for Distance Geometry Problems*, Lectures Notes in Computer Science **6327**, K. Fukuda et al. (Eds.), Proceedings of the 3^{rd} International Congress on Mathematical Software (ICMS10), Kobe, Japan, 186–197, 2010.

54. A. Mucherino, A. Urtubia, *Consistent Biclustering and Applications to Agriculture*, IbaI Conference Proceedings, Proceedings of the Industrial Conference on Data Mining (ICDM10), Workshop on Data Mining in Agriculture (DMA10), Berlin, Germany, 105–113, 2010.

55. A. Mucherino, C. Lavor, L. Liberti, E-G. Talbi, *A Parallel Version of the Branch & Prune Algorithm for the Molecular Distance Geometry Problem*, IEEE Conference Proceedings, ACS/IEEE International Conference on Computer Systems and Applications (AICCSA10), Hammamet, Tunisia, 1–6, 2010.

56. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *An Artificial Backbone of Hydrogens for Finding the Conformation of Protein Molecules*, IEEE Conference Proceedings, Computational Structural Bioinformatics Workshop (CSBW09), International Conference on Bioinformatics & Biomedicine (BIBM09), Washington D.C., USA, 152–155, 2009.

57. A. Mucherino, C. Lavor, *The Branch and Prune Algorithm for the Molecular Distance Geometry Problem with Inexact Distances*, Proceedings of World Academy of Science, Engineering and Technology **58**, International Conference on Bioinformatics and Biomedicine (ICBB09), Venice, Italy, 349–353, 2009.

58. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *Computing Artificial Backbones of Hydrogen Atoms in order to Discover Protein Backbones*, IEEE Conference Proceedings, International Multiconference on Computer Science and Information Technology (IMCSIT09), Workshop on Computational Optimization (WCO09), Mragowo, Poland, 751–756, 2009.

59. A. Mucherino, L. Liberti, C. Lavor, N. Maculan, *Comparisons between an Exact and a MetaHeuristic Algorithm for the Molecular Distance Geometry Problem*, ACM Conference Proceedings, Genetic and Evolutionary Computation Conference (GECCO09), Montréal, Canada, 333–340, 2009.

60. F. Marinelli, O. de Weck, D. Krob, L. Liberti, A. Mucherino, *A General Framework for Combined Module- and Scale-based Product Platform Design*, Electronic Proceedings, 2^{nd} International Symposium on Engineering Systems Proceedings, MIT, Cambridge, Massachusetts, 2009.

61. A.R. Kammerdiner, A. Mucherino, P.M. Pardalos, *Application of Monkey Search Meta-Heuristic to Solving Instances of the Multidimensional Assignment Problem*, Lecture Notes in Control and Information Sciences **381**, M.J. Hirsch, C. Commander, P.M. Pardalos, R. Murphey (Eds.), Proceedings of the 8^{th} International Conference on Optimization and Cooperative Control Strategies (CCO08), Gainesville, Florida, 385–397, 2009.

62. A. Mucherino, O. Seref, *Monkey Search: A Novel Meta-Heuristic Search for Global Optimization*, AIP Conference Proceedings **953**, O. Seref, O.E. Kundakcioglu, P.M. Pardalos (Eds.), Proceedings of the Conference "Data Mining, System Analysis and Optimization in Biomedicine", Gainesville, Florida, 162–173, 2007.

Book chapters (refereed)

63. A. Mucherino, *On the Exact Solution of the Distance Geometry with Interval Distances in Dimension 1*, In: "Recent Advances in Computational Optimization", S. Fidanova (Ed.), Studies in Computational Intelligence **717**, 123–134, 2018.

64. A. Mucherino, S. Fidanova, M. Ganzha, *Introducing the Environment in Ant Colony Optimization*, In: "Recent Advances in Computational Optimization", S. Fidanova (Ed.), Studies in Computational Intelligence **655**, 147–158, 2016.

65. D.S. Gonçalves, J. Nicolas, A. Mucherino, C. Lavor, *Finding Optimal Discretization Orders for Molecular Distance Geometry by Answer Set Programming*. In: "Recent Advances in Computational Optimization", S. Fidanova (Ed.), Studies in Computational Intelligence **610**, 1–15, 2015.

66. J. Seo, J-K. Kim, J. Ryu, C. Lavor, A. Mucherino, D-S. Kim, *BetaMDGP: Protein Structure Determination Algorithm Based on the Beta-complex*. In: "Transactions on Computational Science XXII", M.L. Gavrilova, C.J.K. Tan (Eds.), Lecture Notes in Computer Science **8360**, 130–155, 2014.

67. T.E. Malliavin, A. Mucherino, M. Nilges, *Distance Geometry in Structural Biology: New Perspectives*. In: "Distance Geometry: Theory, Methods and Applications", A. Mucherino, C. Lavor, L. Liberti, N. Maculan (Eds.), 329–350, 2013.

68. L. Liberti, C. Lavor, A. Mucherino, *The Discretizable Molecular Distance Geometry Problem seems Easier on Proteins*. In: "Distance Geometry: Theory, Mathods and Applications", A. Mucherino, C. Lavor, L. Liberti, N. Maculan (Eds.), 47–60, 2013.

69. A. Mucherino, L. Liberti, *A VNS-based Heuristic for Feature Selection in Data Mining*. In: "Hybrid Meta-Heuristics", Studies in Computational Intelligence **434**, E-G. Talbi (Ed.), 353–368, 2013.

70. A. Mucherino, O. Seref, *Modeling and Solving Real Life Global Optimization Problems with Meta-Heuristic Methods*. In: "Advances in Modeling Agricultural Systems", Springer Optimization and Its Applications **25**, P.J. Papajorgji, P.M. Pardalos (Eds.), 403–420, 2008.

71. G. Ceci, A. Mucherino, M. D'Apuzzo, D. di Serafino, S. Costantini, A. Facchiano, G. Colonna, *Computational Methods for Protein Fold Prediction: an Ab-Initio Topological Approach*. In: "Data Mining in Biomedicine", Springer Optimization and Its Applications **7**, P.M. Pardalos, V. Boginski and A. Vazacopoulos (Eds.), 391–429, 2007.

Short conference papers (up to 4 pages, refereed)

72. F. Elain, A. Mucherino, L. Hoyet, R. Kulpa, *Feature Selection in Time-Series Motion Databases*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS18), Workshop on Computational Optimization (WCO18), Poznan, Poland, 245–248, 2018.

73. A. Mucherino, D.S. Gonçalves, A. Bernardin, L. Hoyet, F. Multon, *A Distance-Based Approach for Human Posture Simulations*, IEEE Conference Proceedings, Federated Conference on Computer Science and Information Systems (FedCSIS17), Workshop on Computational Optimization (WCO17), Prague, Czech Republic, 441–444, 2017.

74. R. Alves, A. Cassioli, A. Mucherino, C. Lavor, L. Liberti, *Adaptive Branching in iBP with Clifford Algebra*, Proceedings of Distance Geometry and Applications (DGA13), Manaus, Amazonas, Brazil, 65–69, 2013.

75. V. Costa, A. Mucherino, L.M. Carvalho, N. Maculan, *On the Discretization of iDMDGP instances regarding Protein Side Chains with Rings*, Proceedings of Distance Geometry and Applications (DGA13), Manaus, Amazonas, Brazil, 99–102, 2013.

76. W. Gramacho, D.S. Gonçalves, A. Mucherino, N. Maculan, *A new Algorithm to Finding Discretizable Orderings for Distance Geometry*, Proceedings of Distance Geometry and Applications (DGA13), Manaus, Amazonas, Brazil, 149–152, 2013.

77. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *Finding Low-Energy Homopolymer Conformations by a Discrete Approach*, Proceedings of Global Optimization Workshop 2012 (GOW12), Natal, Brazil, 3–6, 2012.

78. A. Mucherino, I. Wohlers, G.W. Klau, R. Andonov, *Sparsifying Distance Matrices for Protein-Protein Structure Alignments*, Proceedings of the 10^{th} Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW11), Rome, Italy, 211–214, 2011.

79. L. Liberti, B. Masson, C. Lavor, A. Mucherino, *Branch-and-Prune Trees with Bounded Width*, Proceedings of the 10^{th} Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW11), Rome, Italy, 189–193, 2011.

80. A. Mucherino, C. Lavor, L. Liberti, N. Maculan, *Strategies for Solving Distance Geometry Problems with Inexact Distances by Discrete Approaches*, Proceedings of Toulouse Global Optimization 2010 (TOGO10), Toulouse, France, 93–96, 2010.

81. A. Mucherino, C. Lavor, N. Maculan, *The Molecular Distance Geometry Problem Applied to Protein Conformations*, Proceedings of the 8^{th} Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW09), Paris, France, 337–340, 2009.

82. C. Lavor, L. Liberti, A. Mucherino, N. Maculan, *On a Discretizable Subclass of Instances of the Molecular Distance Geometry Problem*, ACM Conference Proceedings, 24^{th} Annual ACM Symposium on Applied Computing (SAC09), Hawaii, USA, 804–805, 2009.

Extended abstracts (refereed)

83. J. Omer, A. Mucherino, *Integer Programming for the Search of a Discretization Order in Distance Geometry Problems*, Proceedings of the conference ROADEF17, Metz, France, February 2017.

84. A. Mucherino, *Discretization Orders and Distance Geometry*, Proceedings of the conference ROADEF15, Marseille, France, February 2015.

85. D.S. Gonçalves, A. Mucherino, *Challenges for Extending Discretizable Molecular Distance Geometry to Interval Data*, Proceedings of Many Faces of Distances (MFD14), Campinas, São Paulo, Brazil, October 2014.

86. D.S. Gonçalves, J. Nicolas, A. Mucherino, *Searching for Optimal Orders for Discretized Distance Geometry*, Proceedings of Many Faces of Distances (MDF14), Campinas, São Paulo, Brazil, October 2014.

87. R. Alves, A. Cassioli, A. Mucherino, C. Lavor, L. Liberti, *The Integration of Clifford Algebra in the iBP algorithm for the DMDGP*, Proceedings of the International Work-Conference on Bioinformatics and Biomedical Engineering (IWBBIO13), Granada, Spain, 745–746, 2013.

88. M. Le Boudic-Jamin, A. Mucherino, R. Andonov, *Modeling Protein Flexibility by Distance Geometry*, Proceedings of the conference ROADEF12, Angers, France, April 2012.

89. L. Liberti, C. Lavor, A. Mucherino, *An Exponential Algorithm for the Discretizable Molecular Distance Geometry Problem is Polynomial on Proteins*, Proceedings of the 7^{th} International Symposium on Bioinformatics Research and Applications (ISBRA11), Book of extended abstracts, pages 40–43, Changsha, China, May 2011.

90. A. Mucherino, C. Lavor, L. Liberti, *The Discretizable Molecular Distance Geometry Problem: from Ideal to Real Instances*, Proceedings of the conference ROADEF11, Saint Etienne, France, March 2011.

91. A. Mucherino, L. Jourdan, E-G. Talbi, *A Heuristic for Biclustering based on a Bilevel Reformulation*, Proceedings of the International Conference on Metaheuristics and Nature Inspired Computing (META10), Djerba, Tunisia, October 2010.

92. A. Mucherino, S. Cafieri, *A New Heuristic Algorithm for Consistent Biclustering*, Proceedings of the EU/MEeting 2010, Lorient, France, June 2010.

93. A. Mucherino, C. Lavor, L. Liberti, E-G. Talbi, *On Suitable Parallel Implementations of the Branch & Prune Algorithm for Distance Geometry*, Proceedings of the Grid5000 Spring School, Lille, France, April 2010.

94. A. Mucherino, C. Lavor, L. Liberti, N. Maculan, *A Discrete Approach for Finding the Conformation of Molecules from NMR Data*, Proceedings of the conference ROADEF10, Toulouse, France, February 2010.

95. C. Lavor, L. Liberti, A. Mucherino, N. Maculan, *Recent Results on the Discretizable Molecular Distance Geometry Problem*, Proceedings of the conference ROADEF09, Nancy, France, 283–284, 2009.

Other

96. M.C. De Cola, A. Mucherino, G. Felici, L. Liberti, *A Branch-and-Prune Algorithm for the Sensor Network Localization Problem*, IASI Technical Report R.4, 2013.

97. L. Liberti, C. Lavor, B. Masson, A. Mucherino, *Polynomial Cases of the Discretizable Molecular Distance Geometry Problem*, arXiv e-print, arXiv:1103.1264v1, March 2011.

98. A. Mucherino, S. Cafieri, *A New Heuristic for Feature Selection by Consistent Biclustering*, arXiv e-print, arXiv:1003.3279v1, March 2010.

99. A. Mucherino, O. Seref, P.M. Pardalos, *Simulating Protein Conformations through Global Optimization*, arXiv e-print, arXiv:0811.3094v1, November 2008.

Theses

100. A. Mucherino, *On the Discretization of Distance Geometry: Theory, Algorithms and Applications*, HDR Monograph, University of Rennes 1. July 17^{th}, 2018.

101. A. Mucherino, *Geometric Aspects in the Simulation of Protein Folding Processes* (in Italian), PhD Thesis, Second University of Naples. December 18^{th}, 2005.

102. A. Mucherino, *Quadratic Optimization: Algorithms and Software for Dense Problems* (in Italian), Master Thesis, Second University of Naples. October 30^{th}, 2001.