

# Antonio Mucherino's Curriculum Vitæ

## Personal

ANTONIO MUCHERINO (born in 1978)

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## Job history and experiences

Current position (since Sep 2011):

- **Assistant Professor**<sup>1</sup> at IRISA, University of Rennes 1, Rennes, France.

Previous positions:

- **Postdoc Researcher**, from Sep 2006 to Aug 2011

<i>time</i>	<i>where</i>	<i>advisor(s)</i>
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

<i>time</i>	<i>where</i>	<i>advisor</i>
10 months	ISA-CNR, Avellino	Angelo Facchiano
10 months	Giovanni Pascale Foundation, Naples	Giovanni Colonna

- **Trainee** (before PhD)

<i>time</i>	<i>where</i>	<i>advisor</i>
3 months	ICAR-CNR, Naples	Marco D'Apuzzo

## Education

- *Since 2009*

On the **Qualification Lists** for “Maître de Conférences”,  
French National University Council (CNU), Section: 27 (computer science).

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<sup>1</sup>Equivalent to *Maître de Conférences* in France.

- *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<sup>th</sup>, 2005. Supervisor: Marco D'Apuzzo.
- *Sep 1997 - Oct 2001*  
**Degree 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<sup>th</sup>, 2001. Supervisor: Marco D'Apuzzo.

## Research interests

- Bioinformatics
- Distance Geometry
- Data Mining
- Meta-Heuristics for Global Optimization
- Protein Folding Simulations
- Parallel Computing

## Research activities

### Distance Geometry Problem

The Distance Geometry Problem (DGP) is the problem of finding the coordinates of a given set of points in the three-dimensional space when some of the relative distances between pairs of such points are known. An interesting application of this problem is to protein conformations. Experiments of Nuclear Magnetic Resonance (NMR) are able to find estimates of the distances between some atoms of the molecule, and the problem of finding the conformation of the protein by using this information is a DGP.

In collaboration with Leo Liberti, Carlile Lavor and Nelson Maculan, I am working on a combinatorial reformulation of the DGP and on a Branch & Prune (BP) algorithm for its solution [1, 2, 3, 4, 5, 6, 7, 8, 13, 16, 20, 22, 24, 25, 26, 27, 29, 30, 31, 32, 33, 34, 37, 41, 42, 45, 46, 47, 48]. The discretization of the problem is possible when some particular assumptions are satisfied. We proposed two reformulations. The first reformulation is based on the structure of protein conformations, and we refer to the reformulated combinatorial problem as the Discretizable Molecular Distance Geometry Problem (DMDGP). More recently, we proposed another reformulation for the DGP which is based on weaker assumptions that are not related to molecular conformations. We named the reformulated problem Discretizable Distance Geometry Problem (DDGP). The DGP is NP-hard, as well as the DMDGP and the DDGP. For solving both combinatorial problems, we employ a Branch & Prune (BP) algorithm, which is strongly based on the combinatorial structure of the two problems.

Recent works have been particularly devoted to the application of the BP algorithm for the solution of instances of the problem containing real NMR data. For example, NMR is not able to provide exact distances but intervals where the actual distances may be contained [31]. A small percentage of provided distances could also be affected by experimental errors, and therefore the set of distances forming an instance of the problem may not be feasible [29, 33]. The distances provided by NMR are usually between pairs of hydrogen atoms only and smaller than 4–5 Å, and hence the number of available distances is rather limited. However, in [6, 13, 32], we found a particular ordering for the hydrogen atoms of protein backbones for which the assumptions for the DMDGP are always

satisfied. In [4], we considered all hydrogen atoms in a molecule and we developed a strategy for automatically reordering such atoms with the aim of satisfying the assumptions for the DDGP. In both approaches, the solution of the two combinatorial problems provides a set of coordinates for the considered hydrogen atoms. Therefore, in [8, 30], we proposed a polynomial algorithm which is able to construct the full-atom conformation of protein backbones from the coordinates of its hydrogen atoms. Finally, we also found a special ordering for the atoms of protein backbones (both hydrogen and non-hydrogen atoms are considered in this case) for which the assumptions for the DMDGP are always satisfied. The main advantages in using this last approach are: all kinds of atoms are considered simultaneously, and the available distances between hydrogen atoms may be either exact or imprecise [25]. Experimental data from NMR can be managed by employing the *interval* BP (*iBP*) algorithm [1], which is an extension of the BP algorithm that is strongly based on this special ordering for the atoms of protein backbones. For the first time, in [24], we were able to solve NMR instances by employing the *iBP* algorithm. We are also working on parallel versions of the BP and *iBP* algorithms [29, 45].

## Data mining

Data mining is the problem of extracting previously unknown, potentially useful and reliable patterns from a given set of data. In collaboration with Panos Pardalos and Petraq Papajorgji, I wrote a book describing the most important data mining techniques [14]. The book also contains many applications of data mining in agriculture and related fields, such as biology and chemistry. This is the first book completely devoted to applications of data mining techniques in these fields.

In collaboration with Sonia Cafieri, Alejandra Urtubia and Leo Liberti, I am 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 describing the samples. Consistent biclusterings can be exploited for performing supervised classifications, as well as for solving feature selection problems. This problem 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 algorithm which is based on the bilevel reformulation [19, 28, 43, 44, 49]. I recently extended in [17] this technique to sets of data containing negative entries.

As we pointed out in our book [14], we found no applications of biclustering in the agricultural field during the preparation of the book. Successively, we applied this technique for studying wine fermentations [18, 28], in order to predict problematic fermentations at the early stages of the process, and we discovered some compounds of wine that may be the cause of problematic fermentations.

## Meta-Heuristics for Global Optimization

Meta-heuristic methods are widely used in optimization, because they are much more flexible and often easier to implement than deterministic methods. During my postdoc at University of Florida, Onur Seref and I worked on a novel meta-heuristic method for global optimization [36, 38, 39]. We named this method Monkey Search (MS), because it is inspired by the behavior of a monkey which climbs trees in its search for food. Rather than a completely new meta-heuristic approach for global optimization, MS can be seen as a general framework (describing the monkey behavior) where other ideas and strategies for global optimization can also be employed. We implemented MS in C programming language for solving particular classes of optimization problems. A version of this software that is independent from the particular problem to be solved is currently under development.

## Protein Folding Simulations

During my PhD in Italy, I mainly worked on the protein folding problem, whose final aim is the identification of a strategy for correlating the known chemical structure of a protein to its three-dimensional conformation. I performed several analyses on protein conformations, where particular attention was given to their geometric features [9, 40]. I also worked on a model for protein simulations which is mainly based on geometric properties of

protein conformations [40, 50]. Differently from other models for protein prediction, the considered model does not rely on chemical and physical forces involved in the folding process, but it rather attempts the simulation of protein conformations by exploiting their geometric properties. Computational experiments proved that the geometric properties of protein conformations play an important rule in the folding process.

## Parallel Computing

There are several applications that require high computing resources. Parallel computing allows to exploit the CPU power of many processors simultaneously for solving difficult problems. There exist parallel computers with different architectures, and the most used parallel computers are nowadays the MIMD machines with distributed memory. I recently developed [29, 45] a parallel version of the BP algorithm which we use for solving the DMDGP (see above). The experimental testing of the parallel algorithm has been performed on the French nation-wide grid infrastructure Grid5000 ([www.grid5000.fr](http://www.grid5000.fr)).

## Organization activities

- responsible of international relationships in the GenScale team of IRISA.
- co-chair of
  - Workshop on Computational Optimization (WCO12), Wroclaw, Poland, September 9–12, 2012.
- international advisory committee member for
  - Data Mining in Agriculture (DMA12), Berlin, Germany, July 20, 2012.
  - Data Mining in Agriculture (DMA11), New York City, USA, September 2, 2011.
- local organizing committee member for
  - Toulouse Global Optimization 2010 (TOGO10), Toulouse, France, August 31 – September 3, 2010.
  - Cologne-Twente Workshop (CTW09) on “Graphs and Combinatorial Optimization”, Paris, France, June 2–4, 2009.
- refereed papers for:
  - *Journal of Global Optimization* (JOGO, Springer);
  - *Optimization Letters* (OPLT, Springer);
  - *Operational Research: An International Journal* (ORIJ, Springer);
  - *Discrete Applied Mathematics* (DAM, Elsevier);
  - *Plant and Soil* (PLSO, Springer);
  - proceedings for conferences: BIOMAT07, CTW09, DMA11.
- participation in scientific projects:
  - *Bayesian inference paradigm: Biology in processors* (Bip:Bip), ANR project, 2012–2017.
  - *Combinatorial Methods to Calculate Protein Structures by Using NMR Data*, State of São Paulo Research Foundation - FAPESP, 2009–2011.
  - *Innovative Problems and Methods in Nonlinear Optimization*, PRIN Project, Italian Ministry of University and Research (MIUR), 2005–2007;

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

- presentation of the organization of undergraduate courses of the Second University of Naples to high school students, 2002–2006.

## 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. CSBW11, BIBM11, Atlanta, GA, USA, November 12–15, 2011.
2. WCO11, FedCSIS11, Szczecin, Poland, September 18–21, 2011.
3. MAS11, Rome, Italy, September 12–14, 2011.
4. DMA11, ICDM11, New York City, USA, September 2, 2011.
5. COCOA11, Zhangjiajie, China, August 4–6, 2011.
6. IFORS11, Melbourne, Australia, July 10–15, 2011.
7. WCGO11, Crete, Greece, July 3–7, 2011 (*two contributions*).
8. CTW11, Frascati, Rome, June 14–16, 2011 (*two contributions*).
9. LSSC11, Sozopol, Bulgaria, June 6–10, 2011.
10. ISBRA11, Changsha, China, May 27–29, 2011.
11. SEA11, Crete, Greece, May 5–7, 2011.
12. ROADEF11, Saint Etienne, France, March 2–4, 2011.
13. IWCP10, BIBM11, Hong Kong, December 18–21, 2010.
14. META10, Djerba, Tunisia, October 27–31, 2010.
15. ICMS10, Kobe, Japan, September 13–17, 2010.
16. TOGO10, Toulouse, France, August 31 – September 3, 2010.
17. DMA10, ICDM10, Berlin, Germany, July 14, 2010.
18. EURO10, Lisbon, Portugal, July 11–14, 2010.
19. DMBIO10, Crete, Greece, July 7–9, 2010.
20. EU/MEeting 2010, Lorient, France, June 2–4, 2010.
21. AICCSA10, Hammamet, Tunisia, May 16–19, 2010.
22. Grid5000 Spring School 2010, Lille, France, April 6–9, 2010.
23. ROADEF10, Toulouse, France, February 24–26, 2010.
24. CSBW09, BIBM09, Washington D.C., USA, November 1–4, 2009.
25. ICBB09, Venice, Italy, October 28–30, 2009.
26. WCO09, IMCSIT09, Mragowo, Poland, October 12–14, 2009.
27. IFIP09, Buenos Aires, Argentina, July 27–31, 2009.
28. GECCO09, Montréal, Canada, July 8–12, 2009.

29. Engineering Systems Symposium at MIT, Cambridge, Massachusetts, USA, June 15–17, 2009.
30. CTW09, Paris, France, June 2–4, 2009.
31. FAME09, Orlando, Florida, USA, May 14–17, 2009.
32. Small group meeting, CIRM, Marseille, France, March 10–12, 2009.
33. SAC09, Honolulu, Hawaii, USA, March 8–12, 2009.
34. ROADEF09, Nancy, France, February 10–12, 2009.
35. BBCC08, Avellino, Italy, December 12, 2008.
36. Workshop “Journée Optimeo”, Université Paris-Sud XI, Orsay, France, November 21, 2008.
37. ARS Workshop, École Polytechnique, Palaiseau, France, October 31, 2008.
38. CCO08, Gainesville, Florida, USA, January 30 - February 1, 2008.
39. Protein Folding Workshop, Minneapolis, USA, January 14–18, 2008.
40. Biomedicine07, Gainesville, Florida, USA, March 28–30, 2007.
41. BBCC06, Avellino, Italy, December 18, 2006.
42. Biomedicine05, Gainesville, Florida, USA, February 2–4, 2005.
43. CMS04, Neuchatel, Switzerland, April 2–5, 2004.
44. Unravelling Nature’s Networks, Sheffield, England, July 20–22, 2003.

## Visiting Terms and Seminars

1. BIA, INRA, Toulouse, France. 1 seminar. Invited by M. Vignes. March 2012.
2. COPPE, Federal University of Rio de Janeiro, Brazil. 15 days, 1 seminar.  
Invited by N. Maculan. August 2011.
3. Universidad Técnica Federico Santa Maria, Valparaíso, Chile. 7 days, 2 seminars.  
Invited by A. Urtubia. July 2011.
4. IMECC, UNICAMP, Campinas, Brazil. 10 days. Invited by C. Lavor. June 2011.
5. LIPN, Université de Paris 13, Paris, France. 1 seminar. Invited by R.W. Calvo. April 2011.
6. LIRMM, Université de Montpellier 2, Montpellier, France. 1 seminar. Invited by O. Gascuel. April 2011.
7. IRIT, Toulouse, France. 1 seminar. Invited by F. Messine. April 2011.
8. LAMIH, Université de Valenciennes, Valenciennes, France. 1 seminar. Invited by S. Hanafi. March 2011.
9. IMECC, UNICAMP, Campinas, Brazil. 15 days. Invited by C. Lavor. July 2010.
10. CERFACS, Toulouse, France. 1 seminar. Invited by I. Duff. June 2010.
11. LRI, Université Paris 11, Orsay, France. 1 seminar. Invited by Ch. Froidevaux. April 2010.
12. Département de Mathématiques et d’Informatique, Université de Reims Champagne-Ardenne,  
Reims, France. 1 seminar. Invited by M. Krajecki. April 2010.
13. LIPADE, Université Paris Descartes, Paris, France. 1 seminar. Invited by M. Nadif. April 2010.
14. IMECC, UNICAMP, Campinas, Brazil. 15 days, 1 seminar. Invited by C. Lavor. March 2010.
15. ENSEEIHT, Toulouse, France. 1 seminar. Invited by P.R. Amestoy. March 2010.
16. IRISA, Rennes, France. 1 seminar. Invited by R. Andonov. December 2009.

17. Université Paris 11, Orsay, France. 1 seminar. Invited by A. Lissier. April 2009.
18. LAMSADE, Université Paris Dauphine, Paris, France. 1 seminar. Invited by A.R. Mahjoub. March 2009.
19. DIIGA, Università Politecnica delle Marche, Ancona, Italy. 1 seminar.  
Invited by F. Marinelli. February 2009.
20. Department of Industrial Engineering, University of Florida, USA. 1 seminar.  
Invited by P.M. Pardalos. January 2007.
21. IASI-CNR, Rome, Italy. 1 seminar. Invited by M. Sciandrone. September 2003.

## Teaching

Only information about the classes I am currently teaching can be found here.

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. **Applied Informatics** (in French, “Informatique Appliquée”).  
*Formation PCSTM*, University of Rennes 1, as teacher.  
Academic year 2011/12, first semester, level L2 (B.Sc).
2. **Programming 1** (in French, “Programmation 1”).  
*Formation INFO*, University of Rennes 1, as teacher.  
Academic year 2011/12, first semester, level L3 (B.Sc).
3. **Network Sizing** (in French, “Dimensionnement des Réseaux”).  
*Formation ESIR*, University of Rennes 1, as teacher.  
Academic year 2011/12, first semester, level M2 (M.Sc).
4. **Operational Research** (in French, “Recherche Opérationnelle”).  
*Formation MIAGE*, University of Rennes 1, as assistant.  
Academic year 2011/12, first semester, level M1 (M.Sc).

Previous courses were given at the École Polytechnique in Palaiseau (France) and at the Second University of Naples (Italy).

## Supervision and tutoring

- Academic years 2010–13: Co-supervision (with C. Lavor) of the PhD thesis of Warley Gramacho.
- Academic year 2005–06: Co-supervision (with M. D’Apuzzo) of the M.Sc. thesis of Giovanni Cicia.
- Academic year 2003–04: Co-supervision (with M. D’Apuzzo) of the M.Sc. thesis of Enrico Raimondo.
- Academic year 2002–03: Co-supervision (with M. D’Apuzzo) of the M.Sc. thesis of Matilde Muto.
- Personal tutor for students of the Second University of Naples from 2003 to 2006.

## Computer-related skills

- Programming Languages: C, C++, Java, Fortran 77/90, PHP, Matlab, Python.
- Operating Systems: UNIX, Linux, Windows 7, Vista, XP.
- Linear Algebra Packages: BLAS, LAPACK.
- Optimization Systems and Software: CPLEX, SNOPT, AMPL and others, both commercial and free.
- Parallel Computing Packages: MPI, SCALAPACK.

## Developed software

### MD-JEEP

*Implementation of:* the Branch and Prune algorithm for the Molecular Distance Geometry Problem

*Programming language:* C

*Description:* This is an implementation of the Branch & Prune (BP) algorithm for the Discretizable Molecular Distance Geometry Problem (DMDGP). MD-JEEP is the result of a strong collaboration among myself, Leo Liberti, Carlile Lavor and Nelson Maculan. Many details regarding the discretization of the problem and the BP algorithm can be found in our publications [1, 2, 3, 4, 5, 6, 7, 8, 13, 16, 20, 22, 24, 25, 27, 29, 30, 31, 32, 33, 34, 37, 41, 42, 45, 46, 47, 48]. Moreover, a recent paper is completely devoted to MD-JEEP [26]. MD-JEEP is distributed under the GNU General Public Licence (v.2). Its sources are available for download at the address: <http://www.antoniomucherino.it/en/mdjeep.php>.

### MS

*Implementation of:* the Meta-Heuristic algorithm 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 [38, 39], the simulation of protein conformations [38, 50], the Multidimensional Assignment Problem (MAP) [36], and the Distance Geometry Problem (DGP) [33].

### AN-PRO

*Implementation of:* Analyses on Protein Conformations

*Programming language:* C

*Description:* This software tool performs various analyses on protein conformations. It is able to read files in `pdb` format (standard format for protein conformations) and in `fasta` format (standard format for amino acid sequences). The results of the analyses are given in `csv` format, which is compatible with Microsoft Excel. Some of the analyses performed by AN-PRO have been published in [9, 40].

## Languages

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

## Publications

### International journals

1. C. Lavor, L. Liberti, A. Mucherino, *The interval Branch-and-Prune Algorithm for the Discretizable Molecular Distance Geometry Problem with Inexact Distances*, to appear in *Journal of Global Optimization*, 2012.
2. C. Lavor, L. Liberti, N. Maculan, A. Mucherino, *Recent Advances on the Discretizable Molecular Distance Geometry Problem*, *European Journal of Operational Research*, available online, 2012.

3. A. Mucherino, C. Lavor, L. Liberti, *The Discretizable Distance Geometry Problem*, Optimization Letters, *Online First Articles*, June 2011.
4. C. Lavor, J. Lee, A. Lee-St. John, L. Liberti, A. Mucherino, M. Sviridenko, *Discretization Orders for Distance Geometry Problems*, Optimization Letters, *Online First Articles*, March 2011.
5. C. Lavor, L. Liberti, N. Maculan, A. Mucherino, *The Discretizable Molecular Distance Geometry Problem*, Computational Optimization and Applications, *Online First Articles*, March 2011.
6. 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.
7. 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.
8. 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.
9. A. Mucherino, A. Masello, *Statistical Analysis on the Globular Shape of Protein Conformations*, JP Journal of Biostatistics **4**(1), 1–12, 2010.
10. 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.
11. A. Mucherino, S. Costantini, D. di Serafino, M. D’Apuzzo, A. Facchiano and 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.
12. 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

13. 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

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

### Edited books

15. S. Cafieri, A. Mucherino, G. Nannicini, F. Tarissan, L. Liberti (Eds.), *Proceedings of the 8<sup>th</sup> Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW09)*, Paris, France, 2009.

### Conference papers (refereed)

16. 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.

17. A. Mucherino, *Extending the Definition of  $\beta$ -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.
18. A. Mucherino, A. Urtubia, *Feature Selection for Datasets of Wine Fermentations*, Proceedings of the 10<sup>th</sup> International Conference on Modeling and Applied Simulation (MAS11), Rome, Italy, 309–313, 2011.
19. A. Mucherino, G. Ruß, *Recent Developments in Data Mining and Agriculture*, IbaI Conference Proceedings, Proceedings of the Industrial Conference on Data Mining (ICDM11), Workshop “Data Mining in Agriculture” (DMA11), New York City, USA, 90–98, 2011.
20. 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<sup>th</sup> Annual International Conference on Combinatorial Optimization and Applications (COCOA11), Zhangjiajie, China, 322–342, 2011.
21. A. Mucherino, I. Wohlers, G.W. Klau, R. Andonov, *Sparsifying Distance Matrices for Protein-Protein Structure Alignments*, Proceedings of the 10<sup>th</sup> Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW11), Rome, Italy, 211–214, 2011.
22. L. Liberti, B. Masson, C. Lavor, A. Mucherino, *Branch-and-Prune Trees with Bounded Width*, Proceedings of the 10<sup>th</sup> Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW11), Rome, Italy, 189–193, 2011.
23. A. Mucherino, M. Fuchs, X. Vasseur, S. Gratton, *Variable Neighborhood Search for Robust Optimization and Applications to Aerodynamics*, to appear in Lecture Notes in Computer Science **7116**, Proceedings of the 8<sup>th</sup> International Conference on Large-Scale Scientific Computations (LSSC11), Sozopol, Bulgaria, June 2011.
24. 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 and S. Rebennack (Eds.), Proceedings of the 10<sup>th</sup> International Symposium on Experimental Algorithms (SEA11), Crete, Greece, 206–217, 2011.
25. 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.
26. 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 Third International Congress on Mathematical Software (ICMS10), Kobe, Japan, 186–197, 2010.
27. 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.
28. A. Mucherino, A. Urtubia, *Consistent Biclustering and Applications to Agriculture*, IbaI Conference Proceedings, Proceedings of the Industrial Conference on Data Mining (ICDM10), Workshop “Data Mining in Agriculture” (DMA10), Berlin, Germany, 105–113, 2010.
29. 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.

30. 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.
31. 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.
32. 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.
33. 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.
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