Antonio Mucherino's Curriculum Vitæ

Personal

Antonio Mucherino (born in 1978)
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Research interests

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

Education

- *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, 2005. Supervisor: Prof. 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, 2001. Supervisor: Prof. Marco D'Apuzzo.

Job history and experiences

Postdoc Researcher, *from Sep 2006 to Present*

1. *INRIA, Lille Nord Europe*, Villeneuve d'Ascq, France.
   Topics: Combinatorial Optimization, Bioinformatics. Research Advisor: Prof. El-Ghazali Talbi.

2. *Laboratoire d'Informatique de l'École Polytechnique* (LIX), Palaiseau Cedex, France (until Oct 2009).
   Topics: Clustering, Distance Geometry Problem, Optimization. Research Advisor: Prof. Leo Liberti.
   Research Co-advisor: Prof. Carlile Lavor (from Sep 2008 to Feb 2009).

3. *Institute of Food and Agricultural Sciences* (IFAS),
   University of Florida, Gainesville, Florida (until May 2008).
   Topics: Data mining, Optimization. Research Advisor: Prof. Petraq Papajorgji.

4. *Center for Applied Optimization* (CAO), University of Florida, Gainesville, Florida (until Jun 2007).
   Topics: Meta-Heuristics for Global Optimization, Protein Folding. Research Advisor: Prof. Panos Pardalos.

5. *Department of Agricultural Engineering and Agronomy*, University of Naples "Federico II",
   Naples, Italy (until Oct 2006).
   Project title: *Development of Software for Nonlinear Optimization*. Research Advisor: Prof. Gerardo Toraldo.

Experiences during the PhD, *from Nov 2001 to Dec 2005*

1. Contract at the *Institute of Food Science* (ISA-CNR), Avellino, Italy (10 months).
   Project title: *Computational Experiences for Protein Folding Simulations*.
   Research Advisor: dr. Angelo Facchiano.

2. Contract at the *Giovanni Pascale Foundation*, Naples, Italy (10 months).
   Project title: *Development of a Web-Learning system for Chemistry, Biochemistry, Mathematics and Medicine*.
   Research Advisor: Prof. Giovanni Colonna.

Previous experiences

1. **Stage** (3 months) at *Center for Research on Parallel Computing and Supercomputers* - CPS/CNR,
   nowadays *Institute for High Performance Computing and Networking* - ICAR/CNR - Naples branch.
   Research Advisor: Prof. Marco D'Apuzzo.

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 the atoms of the molecule which are closer than about 6Å. The problem of finding all the coordinates of the atoms of a protein by using the information on the distances 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 an ad-hoc algorithm for its solution [1, 2, 3, 4, 9, 12, 14, 15, 16, 17, 18, 21, 25, 26, 27, 28]. 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). For solving both the combinatorial problems, we employ a Branch & Prune (BP) algorithm, which is strongly based on the combinatorial structure of the two problems.

We are also working for considering various issues related to NMR experiments. For example, NMR is not able to provide exact distances but intervals where the actual distances may be contained [16]. 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 [14, 18]. Moreover, not all kinds of atoms in a molecule can be considered during NMR experiments, but the obtained distances mainly regard hydrogen atoms. As a consequence, the corresponding problem must be formulated by considering hydrogen atoms only [9, 17]. Then, after the coordinates of the hydrogens of a molecule have been identified, the coordinates of the other atoms could be found by exploiting information known a priori on bond lengths and bond angles [3, 15].

Recent efforts have been devoted to the development of parallel versions of the BP algorithm [14, 25], and to suitable strategies for modifying instances of the DGP so that they satisfy the assumptions for the discretization (submitted paper).

Data mining

Data mining is the problem of extracting previously unknown, potentially useful and reliable patterns from a given set of data. There are various techniques for mining data, and they can be mainly divided into two categories, depending on the fact they exploit (*classification techniques*) or not (*clustering techniques*) information known a priori regarding the data. Most data mining techniques bring to the formulation of a global optimization problem.

In collaboration with Panos Pardalos and Petraq Papajorgji, I wrote a book describing the most used data mining techniques [10]. 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.

I recently started to work 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, and the problem of finding consistent biclusterings of training sets can be formulated as a 0–1 linear fractional optimization problem. I am working on a bilevel reformulation of this optimization problem, and on a heuristic algorithm which is based on the bilevel reformulation [13, 24, 31].

As we pointed out in our book [10], we found no applications of biclustering in the agricultural field during the preparation of the book. In collaboration with Alejandra Urtubia, I recently applied this technique for studying wine fermentations, in order to predict problematic fermentations at the early stages of the process [13].

Meta-Heuristics for Global Optimization

Meta-heuristics methods are widely used in optimization. They are much more flexible and often easier to implement than deterministic methods. On the other side, deterministic methods can guarantee that the solution to the

problem can be found if some assumptions are satisfied, whereas there is only a certain probability that meta-heuristics can find a solution close to the optimal. Meta-heuristic methods are often used in applied fields, such as biology, chemistry and agriculture.

During my post-doc at University of Florida, Onur Seref and I worked on a novel meta-heuristic method for global optimization [20, 22, 29]. We named this method *Monkey Search*, because it is inspired by the behavior of a monkey which climbs trees in its search for food. The trees the monkey explores contain solutions to the optimization problem to be solved, and branches of the tree represent perturbations able to transform one solution into another. At each step, the monkey chooses the branches to climb by applying a random mechanism, which is based on the objective function values of the new corresponding solutions. The monkey prefers better solutions, but it is not forced to choose them.

Rather than a completely new meta-heuristic approach for global optimization, the Monkey Search can be considered as a general framework (describing the monkey behavior) where other ideas and strategies for global optimization are also employed. Perturbations can be taken from other methods for optimization (such as Genetic Algorithms, Harmony Search, Ant Colony Optimization, etc) and other perturbations can also be inspired by the optimization problem to be solved, leading to a wide range of variants for this meta-heuristic method. We implemented the Monkey Search 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 aspects [5, 30]. I also worked on a model for protein simulations which is mainly based on geometric properties of protein conformations [30, 32]. Differently from other models for protein prediction, the considered model does not rely on chemical and physical forces involved into 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 [14, 25] a parallel version of the Branch & Prune algorithm which we use for solving the DMDGP. The experimental testing of the parallel algorithm has been performed on the French nation-wide grid infrastructure Grid5000.

Organization activities

- local organizing committee member for
  - Toulouse Global Optimization workshop (TOGO10), Toulouse, France, August 31st – September 3rd, 2010.
  - Cologne-Twente Workshop (CTW09) on “Graphs and Combinatorial Optimization”, Paris, France, June 2nd–4th, 2009.

- refereed papers for:
  - *Journal of Global Optimization* (JOGO, Springer);
  - *Operational Research: An International Journal* (ORIJ, Springer);
  - *Discrete Applied Mathematics* (DAM, Elsevier);
  - proceedings for conferences: BIOMAT07, CTW09.
- participation in scientific projects:
  - *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, funded by the Italian Ministry of University and Research (MIUR), 2005–2007;
  - *Computational Procedures for Simulating Protein Folding Processes*, funded by the 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

1. The Third International Congress on Mathematical Software (ICMS10).
   Kobe, Japan, September 13 – 17 2010.
   `MD-jeep`*: an Implementation of a Branch & Prune Algorithm for Distance Geometry Problems.*
2. Toulouse Global Optimization 2010 (TOGO10).
   Toulouse, France, August 31 – September 3 2010.
   Strategies for Solving Distance Geometry Problems with Inexact Distances by Discrete Approaches.
3. Workshop on Data Mining and Agriculture (DMA10).
   Berlin, Germany, July 14 2010.
   Consistent Biclustering and Applications to Agriculture.
4. 24^{th} European Conference on Operational Research (EURO10).
   Lisbon, Portugal, July 11–14 2010.
   Discretization of Molecular Distance Geometry Problems by Defining Artificial Orderings on the Molecule.
5. International Conference on Biomedical Data & Knowledge Mining: Towards Biomarker Discovery.
   Crete, Greece, July 7–9 2010.
   Analysing Wine Fermentations by Consistent Biclustering.
6. EU/MEeting 2010 (10^{th} Anniversary of the Metaheuristics Community).
   Lorient, France, June 2–4 2010.
   A New Heuristic Algorithm for Consistent Biclustering.
7. ACS/IEEE International Conference on Computer Systems and Applications (AICCSA10).
   Hammamet, Tunisia, May 16–19 2010.
   A Parallel Version of the Branch & Prune Algorithm for the Molecular Distance Geometry Problem.

8. Grid5000 Spring School 2010.
   Lille, France, April 6–9 2010.
   On Suitable Parallel Implementations of the Branch & Prune Algorithm for Distance Geometry.

9. ROADEF 2010.
   Toulouse, France, February 24–26 2010.
   A Discrete Approach for Finding the Conformation of Molecules from NMR Data.

10. Advanced Methods and Perspectives in Nonlinear Optimization and Control.
    Toulouse, France, February 3–5 2010.
    A New Heuristic for a Linear Fractional 0–1 Optimization Problem for Biclustering.

11. Computational Structural Bioinformatics Workshop (CSBW09).
    Washington D.C., USA, November 1–4, 2009.
    An Artificial Backbone of Hydrogens for Finding the Conformation of Protein Molecules.

12. International Conference on Bioinformatics and Biomedicine (ICBB09).
    Venice, Italy, October 28–30, 2009.
    The Branch and Prune Algorithm for the Molecular Distance Geometry Problem with Inexact Distances.

13. International Multiconference on Computer Science and Information Technology (IMCSIT09).
    Mragowo, Poland, October 12–14, 2009.
    Computing Artificial Backbones of Hydrogen Atoms in order to Discover Protein Backbones.

14. 24^{th} IFIP TC7 Conference on System Modelling and Optimization (IFIP09).
    Buenos Aires, Argentina, July 27–31, 2009.
    The Discretizable Molecular Distance Geometry Problem for Instances Containing Experimental Errors.

15. Genetic and Evolutionary Computation Conference (GECCO09).
    Montréal, Canada, July 8–12, 2009.
    Comparisons between an Exact and a MetaHeuristic Algorithm for the Molecular Distance Geometry Problem.

16. 2^{nd} International Symposium on Engineering Systems.
    MIT, Cambridge, Massachusetts, USA, June 15–17, 2009.
    A General Framework for Combined Module- and Scale-based Product Platform Design.

17. 8^{th} Cologne-Twente Workshop on Graphs and Combinatorial Optimization (CTW09).
    Paris, France, June 2–4, 2009.
    The Molecular Distance Geometry Problem Applied to Protein Conformations.

18. Florida Annual Meeting and Exposition 2009 *Meeting-at-a-Glance* (FAME09).
    Orlando, Florida, USA, May 14–17, 2009.
    Bond Valence Sum (BVS) in FE and MN Complexes: Parameters and Formula Optimization.

19. Meeting on "Modelisation, optimisation et analyse statique".
    CIRM, Marseille, France, March 10–12 2009.
    Monkey Search Meta-Heuristic and Applications.

20. 24^{th} Annual ACM Symposium on Applied Computing (SAC09).
    Honolulu, Hawaii, USA, March 8–12 2009.
    On a Discretizable Subclass of Instances of the Molecular Distance Geometry Problem.

21. ROADEF 2009.
    Nancy, France, February 10–12 2009.
    Recent Results on the Discretizable Molecular Distance Geometry Problem.

22. Bioinformatics and Computational Biology in the Campania Region (BBCC08).
    Avellino, Italy, December 12 2008.
    A Novel Approach for the Molecular Distance Geometry Problem.

23. Workshop "Journée Optimeo".
    Université Paris-Sud XI, Orsay, France, November 21 2008.
    Combinatorial Optimization for the Molecular Distance Geometry Problem.

24. Workshop on Automatic Reformulation Search (ARS).
    École Polytechnique, Palaiseau, France, October 31 2008.
    The Discretizable Molecular Distance Geometry Problem.

25. 8^{th} International Conference on Cooperative Control and Optimization (CCO08).
    Gainesville, Florida, USA, January 30 - February 1 2008.
    Application of Monkey Search Metaheuristics to Solving MAP Instances.

26. Workshop on Protein Folding.
    Minneapolis, USA, January 14–18 2008.
    Simulating Protein Conformations by a Geometric Model.

27. Data Mining, System Analysis and Optimization in Biomedicine.
    Gainesville, Florida, USA, March 28–30 2007.
    A Novel Meta-Heuristic: Monkey Search and Applications on a Geometric Model for Protein Folding.

28. Bioinformatics and Computational Biology in the Campania Region (BBCC06).
    Avellino, Italy, December 18 2006.
    An Ab-Initio Geometric Method for Protein Fold Simulations.

29. Systems Analysis, Data Mining and Optimization in Biomedicine.
    Gainesville, Florida, USA, February 2–4 2005.
    Analising Protein Structural Datasets to get Information on Protein Shapes.

30. Computational Management Science.
    Neuchatel, Switzerland, April 2–5 2004.
    A Geometrical Approach for Protein Secondary Structure Simulations: Computational Issues.

31. Unravelling Nature's Networks: from Microarray and Proteomic Analysis to Systems Biology.
    Sheffield, England, July 20–22 2003.
    Computational Issues of a Topological Approach to Protein Folding.

Visiting Terms and Seminars

1. IMECC, UNICAMP, Campinas, Brazil. 15 days. Invited by C. Lavor. July 2010.

2. CERFACS, Toulouse, France. 1 seminar. Invited by I. Duff. June 2010.

3. LRI, Université Paris 11, Orsay, France. 1 seminar. Invited by Ch. Froidevaux. April 2010.
4. Département de Mathématiques et d'Informatique, Université de Reims Champagne-Ardenne, Reims, France. 1 seminar. Invited by M. Krajecki. April 2010.
5. LIPADE, Université Paris Descartes, Paris, France. 1 seminar. Invited by M. Nadif. April 2010.
6. IMECC, UNICAMP, Campinas, Brazil. 15 days, 1 seminar. Invited by C. Lavor. March 2010.
7. ENSEEIHT, Toulouse, France. 1 seminar. Invited by P.R. Amestoy. March 2010.
8. IRISA, INRIA, Rennes, France. 1 seminar. Invited by R. Andonov. December 2009.
9. Université Paris 11, Orsay, France. 1 seminar. Invited by A. Lisser. April 2009.
10. LAMSADE, Université Paris Dauphine, Paris, France. 1 seminar. Invited by A.R. Mahjoub. March 2009.
11. DIIGA, Università Politecnica delle Marche, Ancona, Italy. 1 seminar. Invited by F. Marinelli. February 2009.
12. Department of Industrial Engineering, University of Florida, USA. 1 seminar. Invited by P.M. Pardalos. January 2007.
13. IASI-CNR, Rome, Italy. 1 seminar. Invited by M. Sciandrone. September 2003.

Teaching experience

Details about the courses can be found on my web site at the address: `http://www.antoniomucherino.it/en/teaching.html`
On the same page, some didactic material can be downloaded.

1. **Introduction to C++** (in French, "Introduction au C++").
   École Polytechnique, Palaiseau, as teacher, academic year 2009/10, first semester, level: M.Sc.
2. **Operations Research** (in French, "Recherche Operationelle").
   École Polytechnique, Palaiseau, as assistant, academic year 2008/09, first semester, level: M.Sc.
3. **Informatics** (in Italian, "Informatica").
   Second University of Naples, as assistant, academic years 2001/05, second semester, level: B.Sc.
4. **Introduction to Numerical Methods for Optimization**
   (in Italian, "Elementi di metodi numerici per l'ottimizzazione").
   Second University of Naples, as assistant, academic year 2005/06, second semester, level: M.Sc.
5. **Parallel Computing** (in Italian, "Calcolo Parallelo").
   Second University of Naples, as assistant, academic years 2002/06, first semester, level: B.Sc.
6. **Numerical Computations** (in Italian, "Calcolo Numerico").
   Second University of Naples, as assistant, academic years 2002/06, second semester, level: B.Sc.
7. **Introduction to Programming** (in Italian, "Laboratorio di Programmazione e Calcolo").
   Second University of Naples, as assistant, academic years 2002/06, second semester, level: B.Sc.

8. **Introduction to Informatics** (in Italian, "Laboratorio di Programmazione").
   Second University of Naples, as assistant, academic years 2002/06, first semester, level: B.Sc.

9. **Introduction to HTML**.
   Second University of Naples, as teacher, academic years 2003/06, mini-course for undergraduate students.

10. **Computational Mathematics** (in Italian, "Matematica Computazionale").
    Second University of Naples, as assistant, academic years 2002/04, first semester, level: M.Sc.

11. **Programming and Numerical Computations** (in Italian, "Calcolo Numerico e Programmazione").
    Second University of Naples, as assistant, academic years 2002/04, second semester, level: M.Sc.

12. **Numerical Analysis** (in Italian, "Analisi Numerica").
    Second University of Naples, as assistant, academic years 2002/05, first semester, level: M.Sc.

Supervision and tutoring

- July 2006: Co-supervision (with M. D'Apuzzo) of the M.Sc. thesis of Giovanni Cicia.
  Topic: Parallel computing for applications related to the protein folding problem.
- July 2004: Co-supervision (with M. D'Apuzzo) of the M.Sc. thesis of Enrico Raimondo.
  Topic: Statistical analyses on protein conformations.
- October 2003: Co-supervision (with M. D'Apuzzo) of the M.Sc. thesis of Matilde Muto.
  Topic: Computational procedures for studying molecular structures.
- Personal tutor for students of the Second University of Naples every academic year from 2003/2004 to 2005/2006.

Computer-related skills

- Programming Languages: C, C++, Fortran 77/90, PHP, Matlab.
- Operating Systems: UNIX, Linux, Windows XP, Vista.
- 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). The algorithm is based on a combinatorial reformulation of the general distance geometry problem. MD-JEEP is the result of a strong collaboration among Antonio Mucherino, 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, 9, 14, 15, 16, 17, 18, 21, 25, 26, 27, 28]. A recent paper is completely devoted to implementation details regarding MD-JEEP [12]. MD-JEEP is distributed under the GNU General Public Licence (v.2). Its sources are available for download from the address: `http://www.antoniomucherino.it/en/mdjeep.php`.

MS

Implementation of: the Meta-Heuristic algorithm Monkey Search
Programming language: C
Description: This software implements the Monkey Search algorithm for global optimization. The software is able to manage different classes of optimization problems. It can consider all the problems in which the optimal clusters of molecules governed by a certain energy function need to be identified [22, 29]. It can also consider all the problems in which a protein conformation is represented by its dihedral angles, and a suitable objective function depending on the dihedral angles needs to be optimized [22, 32]. More recently, the software has been extended for solving DMDGPs [18]. Finally, there is a version of this software developed by Alla Kammerdiner for the Multidimensional Assignment Problem (MAP) [20].

AN–PRO

Implementation of: Analyses on Protein Conformations
Programming language: C
Description: This software performs various analyses on protein conformations. It is able to read files in `pdb` format (standard format for storing conformations of proteins) and in `fasta` format (standard format for storing the sequence of amino acids forming a protein) and to analyze them. The output is given in `csv` format, which is compatible with Microsoft Excel. The majority of the performed analyses regard geometric features of protein molecules. Some of the analyses performed by this software have been published in [30], and, more recently, in [5].

Languages

- Italian: mother tongue.
- English: excellent spoken and written.
- French: intermediate level of knowledge.

Publications

International journals

1. A. Mucherino, C. Lavor, L. Liberti, *The Discretizable Distance Geometry Problem*, Optimization Letters, in revision.

2. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *On the Computation of Protein Backbones by using Artificial Backbones of Hydrogens*, to appear in Journal of Global Optimization, 2010.

3. C. Lavor, A. Mucherino, L. Liberti, N. Maculan, *Discrete Approaches for Solving Molecular Distance Geometry Problems using NMR Data*, to appear in International Journal of Computational Biosciences, 2010.

4. L. Liberti, C. Lavor, A. Mucherino, N. Maculan, *Molecular Distance Geometry Methods: from Continuous to Discrete*, to appear in International Transactions in Operational Research, 2010.

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

6. 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.

7. 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.

8. 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

9. 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.

Books

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

Edited books

11. 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)

12. A. Mucherino, L. Liberti, C. Lavor, `MD-jeep`*: an Implementation of a Branch & Prune Algorithm for Distance Geometry Problems*, Lectures Notes in Computer Science, Proceedings of the Third International Congress on Mathematical Software (ICMS10), Kobe, Japan, September 2010.

13. A. Mucherino, A. Urtubia, *Consistent Biclustering and Applications to Agriculture*, IbaI Conference Proceedings, Workshop on Data Mining and Agriculture, Berlin, Germany, July 2010.

14. 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, May 2010.

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

16. 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.

17. C. Lavor, A. Mucherino, L. Liberti, and 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.

18. A. Mucherino, L. Liberti, C. Lavor, and 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.

19. 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.

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

21. C. Lavor, L. Liberti, A. Mucherino, and 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.

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

Extended abstracts (refereed)

23. A. Mucherino, C. Lavor, L. Liberti, and N. Maculan, *Strategies for Solving Distance Geometry Problems with Inexact Distances by Discrete Approaches*, Proceedings of Toulouse Global Optimization 2010 (TOGO10), Toulouse, France, August/September 2010.

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

25. 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.

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

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