

## **Habilitation Thesis - Summary**

# **Advances in standardized medical informatics and computational molecular dynamics**

*Habilitation Thesis - Summary*

*Dr. Nicolae Goga*

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The image is a screenshot of the news page on the website of the University of Groningen. The header includes the university's logo, name, and founding year (1614), along with navigation links for 'Contact', 'My University', and a search bar. A red navigation bar contains categories like 'Nieuws en agenda', 'Onderwijs', 'Onderzoek', and 'Wetenschap en samenleving'. The main content area features a news article titled 'IEEE-SA Emerging Technology Award received on standardization', dated 10 January 2011. The article text describes Dr. Nicolae Goga's work on standardizing medical device communication protocols. A photograph of a hospital room with medical equipment is shown, with a caption below it. To the right of the photo, there is a short biography of Dr. Goga and his contact information.

rijksuniversiteit groningen 2014 | 400 jaar founded in 1614 - top 100 university Zoek...

Nieuws en agenda Onderwijs Onderzoek Wetenschap en samenleving

Over ons Actueel Nieuws

## Nieuws

- Nieuws doorzoeken
- Nieuwsarchief
- Evenementen en open dagen

### IEEE-SA Emerging Technology Award received on standardization

Datum: 10 januari 2011

Dr. Nicolae Goga (Molecular Dynamics Group, Groningen Biomolecular Sciences and Biotechnology Institute) together with his colleagues from IEEE 11073 Personal Health Devices Working Group were selected to get one of the two 2010 Emerging Technology Awards given by IEEE (Institute of Electrical Engineering).

The award ceremony took place on Sunday December 5<sup>th</sup>, 2010, at the Hyatt Regency Hotel in New York (USA). Dr. Goga is member of the standardization group and co-author of published standard "IEEE Standard 11073-20601™-2008 -Health informatics—Personal health device communication Part 20601: Application profile—Optimized Exchange Protocol".



His work for the standardization group consisted in formally verifying the designs of the transmission protocols between medical devices that send patient-related physiological data and other devices or computer systems that receive those data. Currently, he is working with emeritus professor Herman Berendsen and other specialists from his group on molecular dynamics algorithms, tools and applications.

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Transmission protocols between medical devices that send patient-related physiological data

(see <http://www.rug.nl/news/2011/01/emergingtechnologyaward>)

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# Summary

**Background of the habilitation thesis.** This habilitation thesis describes the scientific contributions of the author from his research performed after his two PhD thesis received from the University of Eindhoven (2004), the Netherlands and University Politehnica of Bucharest (2005), Romania, during almost 10 years of research. Partly it can be summarized by the following quote from the news published on the site of the University of Groningen, the Netherlands, when the author received IEEE Technology Merits Awards, end of 2010:

*Dr. Nicolae Goga together with his colleagues from IEEE 11073 Personal Health Devices Working Group were selected to get one of the two 2010 Emerging Technology Awards given by IEEE (Institute of Electrical and Electronic Engineering).*

*His work for the standardization group consisted in formally verifying the designs of the transmission protocols between medical devices that send patient-related physiological data and other devices or computer systems that receive those data. Currently, he is working with emeritus professor Herman Berendsen and other specialists from his group on molecular dynamics algorithms, tools and applications. (IEEE-SA Emerging Technology Award received on standardization, Faculty of Natural Sciences News, University of Groningen, 10 January 2011, Available online at: <http://www.rug.nl/news/2011/01/emergingtechnologyaward>)*

This thesis describes scientific contributions from the field of bio-informatics, namely medical informatics and computational molecular dynamics. It is true that the two fields intersect only on the level of the domain (bio-informatics). However, because the author has international recognized contributions in the two fields during his research years, we decided to presents both lines of research in this thesis.

**Impact of the research work.** The author of the habilitation thesis is part of the ISO/IEEE 11073 standardization group. Based on the results of the formal work, he is co-authoring the ISO/IEEE 11073- 20601 standard. He is co-authoring also other 8 standards from this family<sup>1</sup>. Impact of this research can be evaluated as world-wide, given the fact that this family of

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<sup>1</sup> IEEE 11073Device Specialization; standards: 1) 10420:2010; 2) 10421:2010; 3) 10472-2010 4) 20601a-2010; 5) 00103-2012; 6) 10406-2011; 7) 10417-2011; 8) 10441:2013;

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standards is an ISO family and it is implemented by powerful companies from all continents such as Philips, Siemens, Intel, IBM, etc., to mention just a few.

The new stochastic algorithm presented in this thesis (Chapter 5) is already part of the new 5.0 version of Gromacs ([www.gromacs.org](http://www.gromacs.org)). Some other new algorithms presented in this thesis (dissipative particle dynamics algorithms, Chapter 5) are in work to be included in the next versions of Gromacs. In this way, MD work presented in this thesis is going to be used world-wide by top scientific groups, having also a world-wide impact.

**Structure of the thesis.** Before going further we need to say two things. First, as we already mentioned, MD is an interdisciplinary field. With two exceptions (Chapters 3 and 5) we tried to concentrate on the computational aspects of the MD contributions of the author. However author had several contributions in the MD theory itself for the development of the new algorithms that are implemented in Gromacs, contributions that are at the intersection of physics with chemistry. With the mentioned exceptions, we did not allocate space to the MD theory itself, but we tried to summarize the new implemented algorithms and concentrate on the computational aspects, making references for further reading to the published articles. However, to give some impression regarding the developed theory, Chapter 3 and Chapter 5 summarize theoretical and results contributions from the field of MD.

With those being said, bellow we give an overview of the different chapters of the thesis and their content.

- Chapter 1 presents the contributions of the author for the formal analysis of ISO/IEEE 11073 20601 standard – contributions included in this standard. Work was published in *Systems Conference, 2009 3rd Annual IEEE*.
- Chapter 2 describes a new method for pulse determination using video-cameras. Work was published in *Bioinformatics and Bioengineering Conference (BIBE), 2013, 13th Annual IEEE*.
- Chapter 3 describes advances in multi-scaling MD modeling. Work was published in the book “*ADVANCES IN PLANAR LIPID BILAYERS AND LIPOSOMES*”, vol. 15, Academic Press, Elsevier Inc, 2012.
- Chapter 4 presents the MPI implementation of one of the algorithms outlined in Chapter 3. Work was published in *Systems Conference, 2009 3rd Annual IEEE*.
- Chapter 5 describes new stochastic and dissipative particles dynamics (DPD) thermostats MD algorithms – work published in *Journal of Chemical Theory and Computation, vol. 8,*

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no. 10, 3637–3649, 2012.

- Chapter 6 discusses the NVIDIA parallelization of the DPD thermostats presented in Chapter 5 – work published in *IEEE 12th International Conference on Bioinformatics & Bioengineering (BIBE), 2012 Annual IEEE*
- .Chapter 7 presents the MPI parallelization of a variant from the DPD algorithms presented in Chapter 5 – published in *Journal of Atomic and Molecular Physics, Volume 2013 (2013), Article ID 579696, 6 pages, 2013.*
- Chapter 8 presents the conclusions.