

MINDAUGAS MARGELEVIČIUS
Institute of biotechnology
Life Sciences Center
Vilnius University
Saulėtekio av. 7
10257 Vilnius, Lithuania
Tel.: +370 682 16532
E-mail: mindaugas.margelevicius@bti.vu.lt

Education

Doctor in Computer Science (Physical sciences), Kaunas University of Technology, Kaunas, September 2002. (Diploma: No. 018694, Vilnius, 10/18/2002).

Field: Theory of diffraction field distribution, mathematical modeling of diffracted electromagnetic energy, optimization methods for diffracted energy landscape.

Dissertation: “Inverse Modeling of Amplitude and Phase Diffraction Gratings”. Adviser: Prof. Habil. Dr. H. Pranevičius; committee members: Prof. Dr. V. Grigaliūnas, Prof. Habil. Dr. J. Mockus, Prof. Habil. Dr. J. Dudonis, Prof. Habil. Dr. K. Kazlauskas.

Master of Computer Science (with honors), Kaunas University of Technology, June 1999.

Field: Computational analysis and processing of diffraction images.

Thesis: “Research of diffraction images and development of computerized methods for their analysis”. Adviser: Prof. Dr. V. Grigaliūnas.

Bachelor of Computer Science, Kaunas University of Technology, May 1997. Work: Design and implementation of an e-mail server-client system.

Finished reinforced gymnasium (secondary school) “Saulės” in Kaunas and extramural physics school “Fotonas” of Šiauliai University in Šiauliai, 1994.

General research interests

Mathematical modeling, mathematical statistics, optimization methods, machine learning, computer algorithms; and their application.

Applied research interests

Biological sequence and structure analysis, sequence and profile alignment, protein remote homology and structure search, protein structure prediction, homology modeling; development of computational methods and their application in bioinformatics.

Teaching

Bioinformatics and Theory of algorithms taught in the past.

Academic positions

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|---|----------------------------|
| Senior research scientist, Institute of Biotechnology | 2006- |
| Researcher, Institute of Biotechnology | 2003-2006, 09/2017-09/2018 |
| Research: Biological sequence and structure analysis, development of computer algorithms and statistical methods and their application to structure, function, and evolution studies. | |
| Lecturer, Kaunas University of Technology | 2002-2006 |
| Courses: Bioinformatics (2006); Theory of algorithms (2002-2006). | |

Research projects (principal investigator)

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| European Regional Development Fund | 2018-2022 |
| “A system of RESTful web services for protein remote homology search in real time and protein modeling” (01.2.2-LMT-K-718-01-0028). 2014-2020 European Union investment in Lithuania: | |

“Research projects implemented by world-class researcher groups”; EUR 289,314. PI: Dr. M. Margelevičius.

Competitive research funding by the Research Council of Lithuania 2013-2015

“Bayesian nonparametrics for detection of distant protein homology” (MIP-049/2013). Activity: “Research teams’ projects”; funded: EUR 99,600. PI: Dr. M. Margelevičius.

Financial support for the publication of research results. (2018) No. P-PUB-18-12; EUR 300. M. Margelevičius.

Financial support for the publication of research results. (2016) No. PUB-16024; EUR 300. M. Margelevičius.

Competitive research funding by the Research Council of Lithuania 2011-2012

“CONDOR: an advanced protein homology detection method“ (MIP-055/2011). Activity: “Research teams’ projects”; funded: Lt 127,000. PI: Dr. M. Margelevičius.

Research projects (participated)

European Union Structural Funds 2013-2015

“Making use of large-scale biological data for the development of a new method to assess protein models and for studying DNA replication and repair systems in bacteria and viruses” (VP1-3.1-ŠMM-07-K-03-004). Global grant measure: “Support for scientific research by scientists and other researchers”. PI: Dr. Č. Venclovas.

Competitive research funding by the Research Council of Lithuania 2010-2011

“The Crystallography Open Database for small molecules“ (MIP-10482). Activity: “Research teams’ projects”. PI: Dr. S. Gražulis.

Howard Hughes Medical Institute 2006-2010
International Research Programme

“Structural characterization of protein interactions in DNA replication, repair and recombination processes through molecular modeling” (55005627). PI: Dr. Č. Venclovas.

Lithuanian state science and studies foundation 2008-2010
High-Technology Development programme

“Structural and functional studies of T4 phage replisome” (C-01/2008/2). PI: Prof. V. Šikšnys.

Lithuanian state science and studies foundation 2009

“Interactive web server for protein homology search and structure prediction” (T-09281). PI: Dr. Č. Venclovas.

Lithuanian state science and studies foundation 2008

„Assessing protein sequence alignment by using structural models“ (T-08218). PI: Dr. Č. Venclovas.

Lithuanian state science and studies foundation 2007

„Development of computational method for remote homology detection between protein sequence families“ (T-07065). PI: Dr. Č. Venclovas.

European Commission Framework programme 6, Marie Curie actions 2004-2006

“Molecular modeling-based characterization of protein complexes involved in DNA repair” (MIRG-CT-2004-004543). PI: Dr. Č. Venclovas.

Howard Hughes Medical Institute 2004-2005
International Research Programme

“Development, testing, and application of comparative protein structure prediction methods with the aim of rendering comparative modeling more robust in the distant homology regime” (55000341). PI: Dr. Č. Venclovas.

European Commission Framework programme 5, 2004-2005
Access to Research Infrastructures (ARI)

”Fold recognition using sequence-derived properties” (HPRI-CT-2001-00153). Coordinator: The Swedish University of Agricultural Sciences.

Fellowships, visits

- Department of Plant Physiology, Umea University, Umea, Sweden 8/20-9/18, 2010
 Strengthening and Sustaining the European Perspectives of Molecular Biotechnology in Lithuania (MoBiLi) under EC Framework programme 7.
- University of Bologna, Bologna, Italy 2/11-2/15, 2008
 The Bologna 9th winter school: “Grand challenges in computational biology”.
- The Linnaeus Centre for Bioinformatics, Uppsala University, Uppsala, Sweden, 05/10-06/11, 2004
 Research project: “Fold recognition using sequence-derived properties” under EC Framework programme 5, Access to Research Infrastructures (ARI).
- School of Life Sciences Research at the University of Dundee, Dundee, Scotland, UK 06/15-06/17, 2004
- Institute of Biomedical and Life Sciences at the University of Glasgow, Glasgow, Scotland, UK 06/15-06/17, 2004
- Medical Research Council Human Genetics Unit, Edinburgh, Scotland, UK 06/15-06/17, 2004
 British Council's project “Crossroads for Ideas” (2004).

Editorship

- Guest Associate Editor, *Frontiers in Bioinformatics* 2022-
 Editing research topic “Advances in nucleic acid and protein sequence analysis”
<https://www.frontiersin.org/research-topics/37645/advances-in-nucleic-acid-and-protein-sequence-analysis>.

Expert activities

Peer-reviewing scientific papers for bioinformatics and machine learning: Journals: *PloS Computational Biology*, *Bioinformatics*, *IEEE Transactions on Parallel and Distributed Systems*, *Computational and Mathematical Methods in Medicine*, *IEEE Access*; Conference proceedings: World Multi-Conference on Systemics, Cybernetics and Informatics WMSCI 2019-2021.

Lithuanian Business Support Agency Expert Reviewer, European Structural and Investment Funds (2020-).

Expert Reviewer, National Science Centre, Poland (2021-).

Awards and achievements

Member of the two-people group winning (TBM category) the community-wide experiment Critical Assessment of Techniques for Protein Structure Prediction, CASP8 , 2008.

Member of the two-people group ranked 2nd (TBM category) in the community-wide experiment Critical Assessment of Techniques for Protein Structure Prediction, CASP6 , 2004.

Lithuania's representative for bio-sciences and participant in the British Council's project “Crossroads for Ideas”, 2004.

Publications

1. Dapkūnas J., Margelevičius M. (2022) The COMER web server for protein analysis by homology. Submitted to *Bioinformatics*.
2. Margelevičius M. (2022) ROPIUS0: A deep learning-based protocol for protein structure prediction and model selection and its performance in CASP14. *bioRxiv*. DOI: 10.1101/2021.06.22.449457.
3. Margelevičius M. (2020) COMER2: GPU-accelerated sensitive and specific homology searches. *Bioinformatics* 36(11), 3570-3572. DOI: 10.1093/bioinformatics/btaa185.
4. Margelevičius M. (2019) Estimating statistical significance of local protein profile-profile alignments. *BMC Bioinformatics* 20, 419. DOI: 10.1186/s12859-019-2913-3.
5. Margelevičius M. (2018) A low-complexity add-on score for protein remote homology search with COMER. *Bioinformatics* 34(12), 2037-2045. DOI: 10.1093/bioinformatics/bty048.

6. Dapkūnas J., Timinskas A., Olechnovič K., Margelevičius M., Dičiūnas R., Venclovas Č. (2017) The PPI3D web server for searching, analyzing and modeling protein-protein interactions in the context of 3D structures. *Bioinformatics* 33(6), 935–937. DOI: 10.1093/bioinformatics/btw756.
7. Margelevičius M. (2016) Bayesian nonparametrics in protein remote homology search. *Bioinformatics* 32(18), 2744–2752. DOI: 10.1093/bioinformatics/btw213.
8. Olechnovič K., Margelevičius M., Venclovas Č. (2011) Voroprot: an interactive tool for the analysis and visualization of complex geometric features of protein structure. *Bioinformatics* 27(5), 723–724. DOI: 10.1093/bioinformatics/btq720.
9. Laganeckas M., Margelevičius M., Venclovas Č. (2011) Identification of new homologs of PD-(D/E)XK nucleases by support vector machines trained on data derived from profile-profile alignments. *Nucleic Acids Res.* 39(4), 1187–1196. DOI: 10.1093/nar/gkq958.
10. Margelevičius M., Laganeckas M., Venclovas Č. (2010) COMA server for protein distant homology search. *Bioinformatics* 26(15), 1905–1906. DOI: 10.1093/bioinformatics/btq306.
11. Margelevičius M., Venclovas Č. (2010) Detection of distant evolutionary relationships between protein families using theory of sequence profile-profile comparison. *BMC Bioinformatics* 11, 89. DOI: 10.1186/1471-2105-11-89.
12. Venclovas Č., Margelevičius M. (2009) The use of automatic tools and human expertise in template-based modeling of CASP8 target proteins. *Proteins* 77 (Suppl 9), 81–88. DOI: 10.1002/prot.22515.
13. Repšys V., Margelevičius M., Venclovas Č. (2008) Re-searcher: a system for recurrent detection of homologous protein sequences. *BMC Bioinformatics* 9, 296. DOI: 10.1186/1471-2105-9-296.
14. Rudokaitė-Margelevičienė D., Pranevičius H., Margelevičius M. (2006) Data classification using Dirichlet mixtures. *Information Technology and Control*, 35(2), 157–166. ISSN 1392-124X. [VINITI; INSPEC]
15. Venclovas Č., Margelevičius M. (2005) Comparative modeling in CASP6 using consensus approach to template selection, sequence-structure alignment and structure assessment. *Proteins* 61(Suppl 7), 99–105. DOI: 10.1002/prot.20725.
16. Margelevičius M., Venclovas Č. (2005) PSI-BLAST-ISS: an intermediate sequence search tool for estimation of the position-specific alignment reliability. *BMC Bioinformatics* 6, 185. DOI: 10.1186/1471-2105-6-185.
17. Margelevičius M., Grigaliūnas V., Pranevičius H., Margelevičius J. (2003) Modelling of relief of phase reflection diffraction grating. *Appl. Math. Modelling* 27(12), 1035–1049. DOI: 10.1016/S0307-904X(03)00137-9.
18. Margelevičius M., Margelevičius J. (2003) Object specification of a diffraction system. *Information technology and control* 27(2), 69–74. ISSN 1392-124X.
19. Margelevičius M., Timinskas A. (2003) PSI-BLAST algoritmo efektyvumas priklausomybėje nuo skenavimo lango dydžio [Effectiveness of the PSI BLAST algorithm in dependence on scanning word size]. *Liet. matem. Rink.* 43, 532–537. ISSN 0132-2818. [MathSciNet; Zentralblatt MATH (zbMATH); CIS: Current Index to Statistics]
20. Margelevičius M. (2002) Inverse modeling of phase diffraction gratings estimating intensities programmically. *Information technology and control* 23(2), 69–76. ISSN 1392-124X.
21. Grigaliūnas V., Kopustinskas V., Meškiniš Š., Margelevičius M., Mikulskas I., Tomašiūnas R. (2001) Replication technology for photonic band gap applications. *Optical Materials* 17(1-2), 15–18. DOI: 10.1016/S0925-3467(01)00073-8.
22. Kopustinskas V., Grigaliūnas V., Jucius D., Meškiniš Š., Margelevičius M., Tomašiūnas R. (2001) α -C:H films for photonic structures fabrication. *Proc. SPIE* 4318, 295–300. DOI: 10.1117/12.417614.
23. Margelevičius M., Grigaliūnas V., Pranevičius H. (2001) Modeling of lamellar transmission diffraction grating by solving the reverse diffraction problem. *Information technology and control* 18(1), 52–59. ISSN 1392-124X.
24. Kopustinskas V., Grigaliūnas V., Meškiniš Š., Margelevičius M., Tomašiūnas R. (2000) Formation of photonic band gap crystal by SF₆ reactive ion beam etching. *Lithuanian Journal of Physics* 40(1-3), 140–143. ISSN 1392-1932. [Chemical Abstracts (CAplus)]
25. Jucius D., Grigaliūnas V., Margelevičius M. (2000) Submikroninių litografinių darinių optinių savybių tyrimas [Investigation of optical properties of submicrometer lithographic structures]. *Elektronika ir*

elektrotechnika [Electronics and Electrical Engineering] 27(4), 22–27. ISSN 1392-1215. [Chemical Abstracts (CAplus)]

Conference proceedings

1. Rudokaitė-Margelevičienė D., Pranevičius H., Margelevičius M. Plataus taikymo autonominio apmokymo įrankis duomenų klasifikavimui [A machine learning tool of wide applicability for data classification]. *Informacinės technologijos 2006* : konferencijos pranešimų medžiaga / Kauno technologijos universitetas. T. 2. Kaunas : Technologija, 2006. ISBN 9955099933. p. 693-699.
2. Margelevičius M. Difrakcijos gardelių geometrijos matavimas skaterometrijos principu [Measuring the geometry of diffraction gratings using laser scatterometry]. *Informacinės technologijos 2001* : konferencijos pranešimų medžiaga / Kauno technologijos universitetas. Kaunas : Technologija, 2001. ISBN 9955090987. p. 246-250.
3. Grigaliūnas V., Kopustinskas V., Jucius D., Meškiniš Š., Margelevičius M. Fotoninių struktūrų replikavimo metodas [A method for replicating photonic band-gap structures]. *Taikomoji fizika* : konferencijos pranešimų medžiaga, Kaunas, 2000 m. balandžio 13. Kaunas : Technologija. 2000, p. 263-266.
4. Margelevičius M., Grigaliūnas V. Periodinių mikrostruktūrų nanometrologijos ypatumai [Nanometrology of periodic microstructures]. *Informacinės technologijos '2000* : konferencijos pranešimų medžiaga. Kaunas : Technologija, 2000. ISBN 9986138264. p. 198-202.
5. Grigaliūnas V., Kopustinskas V., Gudaitis R., Margelevičius M. DOE formavimo reaktyviųjų jonų pluoštu SF6 dujose ypatumai [Properties of DOE formation by ion beam etching in SF6 gas]. *Spinduliūtės ir medžiagos sąveika* : konferencijos pranešimų medžiaga. Kaunas : Technologija. 1999, p. 98-104.
6. Grigaliūnas V., Margelevičius M. Programinė įranga difrakcinių vaizdų analizei [Software for analysis of diffraction images]. *Informacinės technologijos '99* : konferencijos pranešimų medžiaga / Kauno technologijos universitetas. Kaunas : Technologija, 1999. ISBN 9986137187. p. 67-72.
7. Margelevičius M., Grigaliūnas V., Margelevičius J. Difrakcinių optinių elementų efektyvumo tyrimas [Efficiency analysis of diffractive optical elements]. Pirmoji respublikinė jaunųjų mokslininkų konferencija "Lietuva be mokslo - Lietuva be ateities". Vilnius : Technika. 1998, p. 42-52.
8. Margelevičius M., Andrulevičius M. Mikroreljefinių struktūrų tyrimas optiniais-skaitmeniniais metodais [Analysis of microrelief structures by optical-numerical methods]. *Informacinės technologijos '98* : konferencijos pranešimų medžiaga. Kaunas : Technologija, 1998. ISBN 9986135974. p. 276-279.

Software published

COMER web server backend. COMER web server backend module for protein analysis by homology. Margelevičius M. (2021). [<https://github.com/minmarg/comer-ws-backend>; <https://bioinformatics.lt/comer>]

COTHER. COTHER, a protein remote homology search and threading tool. Margelevičius M. (2021). [<https://github.com/minmarg/cother>]

ROPIUS0. ROPIUS0: A deep learning-based protocol for protein structure prediction and model selection. Margelevičius M. (2021). [<https://github.com/minmarg/ropius0>]

COMER2. COMER2, a cross-platform software package for protein remote homology search and alignment on the GPU. Margelevičius M. (2019). [<https://github.com/minmarg/comer2>]

COMER. Protein remote homology detection and search and profile alignment. Margelevičius M. (2016) *Bioinformatics* 32(18), 2744–2752; Margelevičius M. (2018) *Bioinformatics* 34(12), 2037–2045; Margelevičius M. (2019) *BMC Bioinformatics* 20, 419. [<https://github.com/minmarg/comer>]

PPI3D. Prediction and modeling of protein-protein interactions. Dapkūnas J. et al. (2017) *Bioinformatics* 33(6), 935–937.

Voroprot. Environment for protein structure analysis. Olechnovič K. et al. (2011) *Bioinformatics* 27(5), 723–724.

PDEXK. Restriction endonuclease (protein/enzyme) recognition. Laganeckas M. et al. (2011) *Nucleic Acids Res.* 39(4), 1187-1196.

COMA web server. Web services for COMA search and protein modeling. Margelevičius M. et al. (2010) *Bioinformatics* 26(15), 1905-1906.

COMA. Protein homology search assisted with the estimation of statistical significance. Margelevičius M. et al. (2010) *BMC Bioinformatics* 11, 89. [<https://github.com/minmarg/coma>]

Re-searcher. Web service for an inspection for homology of protein sequences of interest. Repšys V. et al. (2008) *BMC Bioinformatics* 9, 296.

PSI-BLAST-ISS. Reliability assessment of protein multiple sequence alignments. Margelevičius M. et al. (2005) *BMC Bioinformatics* 6, 185.

DIFFRAIN. Environment for analysis of diffraction images and calculation of diffraction intensities. Margelevičius M. et al. (2003) *Appl. Math. Modelling* 27(12), 1035-1049.

International Conferences

Dapkūnas J. and Margelevičius M. (2021) Protein analysis web service powered by the COMER2 homology search engine, [poster]. ISMB/ECCB 2021, July 25-30, 2021, Virtual Symposium.

Margelevičius M. (2020) MSA, the language to translate, [Deep learning roundtable discussions]. CASP14, Nov 30-Dec 04, 2020, CASP14 Virtual Symposium.

Margelevičius M. (2020) ROPIUS0: Restraint-Oriented Protocol for Inference and Understanding of protein Structures, [poster]. CASP14, Nov 30-Dec 04, 2020, CASP14 Virtual Symposium.

Margelevičius M. (2019) Fast homology search with COMER, [poster]. GCB 2019, Sep 16-19, 2019, Heidelberg, Germany.

Dapkūnas J. and Margelevičius M. (2019) A multipurpose web service for protein analysis based on the remote homology search method COMER running on GPU, [poster]. GCB 2019, Sep 16-19, 2019, Heidelberg, Germany.

Margelevičius M. (2018) Estimating statistical significance of protein profile-profile alignments, [poster]. ECCB 2018, Sep 9-12, 2018, Athens, Greece.

Margelevičius M. (2014) CASP11; Protein Structure Prediction Center; Dec 7-10, 2014, Riviera Maya, Mexico.

Margelevičius M., Venclovas Č. (2012) A t-distribution-based scoring of sequence profile pair in protein distant homology search, [poster]. CASP10; Protein Structure Prediction Center; Dec 9-12, 2012, Gaeta, Italy.

Margelevičius M., Venclovas Č. (2012) A t-distribution-based scoring of sequence profile pairs in protein distant homology search, [poster]. ECCB 2012, Sep 9-12, 2012, Basel, Switzerland.

Margelevičius M., Laganeckas M., Venclovas Č. (2010) COMA server for protein distant homology search, [poster]. ECCB 2010, Sep 26-29, 2010, Ghent, Belgium.

Margelevičius M., Venclovas Č. (2008) COMA: a novel protein homology detection method based on the analytical theory of profile comparisons, [poster]. CASP8; Protein Structure Prediction Center; Dec 3-7, 2004, Quartu S. Elena, Sardinia, Italy.

Margelevičius M., Venclovas Č. (2008) A novel protein homology detection method based on the analytical theory of profile comparisons [poster]. ECCB'08; ISCB; Sep 22-26, 2008, Cagliari, Sardinia, Italy.

Margelevičius M., Venclovas Č. (2008) A novel protein homology detection method based on the analytical theory of profile comparisons [poster]. Bioinformatics 2008; SocBiN; Apr 24-27, 2008, Warsaw, Poland.

Margelevičius M., Venclovas Č. (2007) Comparison of the empirical and analytical approaches for the estimation of statistical significance in sequence profile-profile comparisons, [poster]. ECCB 2006, Jan 21-24, 2007, Eilat, Israel.

Margelevičius M., Venclovas Č. (2006) A new approach for estimation of statistical significance in sequence profile-profile comparisons, [poster]. BIOINFORMATICS 2006, June 15-18, 2006, Aarhus, Denmark.

Margelevičius M., Venclovas Č. (2006) A Psi-Blast based tool to assess alignment reliability through an intermediate sequence search, [poster]. RECOMB-2006, Apr 2-5, 2006, Venice, Italy.

Margelevičius M., Venclovas Č. (2005) PSI-BLAST-ISS, intermediate sequence searching for estimation of sequence alignment reliability, [poster]. ISMB-2005, July 25-29, 2005, Detroit, MI.

Margelevičius M., Venclovas Č. (2004) PSI-BLAST-ISS: an intermediate sequence search tool for estimation of position-specific alignment reliability, [poster]. CASP6; CASP6 Organizing Committee; Dec 4-8, 2004, Gaeta, Italy.

Margelevičius M. (2004) The PSI-BLAST Intermediate Sequence Search tool for estimation of position-specific alignment reliability, [talk]. SAC-CASP6; CASP6 Organisers; Dec 3-4, 2004, Gaeta, Italy.

Margelevičius M. (2004) Fold recognition using descriptor data, [talk]. Crossroads for Ideas: Bio-sciences workshop, June 15-18, 2004; British Council; Edinburgh; Scotland, UK.

Margelevičius M. (2005) Patikimų išlygiavimo rėžių identifikavimas baltymų sekų palyginiuose [Identification of reliable alignment boundaries in protein sequence alignments]. Invited talk, the 8th Lithuanian young researchers conference “Science – The Future of Lithuania”; Apr 14, 2005, VGTU, Vilnius.

Margelevičius M., Timinskas A. (2003) PSI-Blast algoritmo efektyvumas priklausomybėje nuo skenavimo lango dydžio [Effectiveness of the PSI BLAST algorithm in dependence on scanning word size], [talk]. 44th conference organized by Lithuanian Mathematical Society, Jun 19-20, 2003, VPU, Vilnius.

Industrial experience

Sen. programmer-engineer, ELSIS Inc. 1999-2002

Responsibilities: Software design and development for the analogous telephone exchange STS16. Real-time software design, development, and installation on the controllers of the digital telephone exchanges NOKIA 210/220 (versions R3 and R4) installed in Saint Petersburg (Russia).

Programmer-engineer, Lietuvos energija Inc. [Lithuanian Energy] 1998-1999

Responsibilities: Database design and development for citizens' electricity consumption.

Work by Contract 1997-1998

Service of Technological Security of State Documents under the Ministry of Finance

Responsibilities: Development of computational method and software for controlling the quality of diffractive optical elements for document security.

Computer skills

Operating systems: UNIX family systems: Linux, IRIX, QNX, Neutrino, Sun Solaris; MS Windows.

Programming languages: C, C++ (1995-), CUDA C++, Perl, R, Matlab, Python, Java, XML, Vbasic, SQL, LISP, Prolog, ASM, Delphi; MySQL, Oracle (as DBMSs).

Technologies: CUDA, MPI, Grid Computing, .NET, J2EE, CORBA, OLE, DDE.

Other

Languages: Lithuanian (native), English (good), Russian (good).