Curriculum vitæ Vedran Miletić

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Core skills

***In silico* drug design and software development**	Scientific software development and research experience in **computational biochemistry**, **molecular modeling**, and its applications to *in silico* drug design **GROMACS**: porting AMBER ff14SB and ff19SB; developed **conditional stopping** and **solvent acceleration** features, improved developer experience, contributed over 140 patches in total (C/C++, MPI, CUDA/OpenCL/SYCL, Python, CMake, Git) **RxDock**, a fork of **rDock**: led the project, more than 100 commits in 3 years as scientific software architect at **RxTx Research** (C++, Eigen, {fmt}, JSON, Meson)
Network and system administration	Planning, installation, configuration, and maintenance of **application-** and **network-layer services** on Linux and FreeBSD in **bare metal** and **virtualized** environments (including **containers**), installation and configuration **automation**; experience with network emulation and simulation (ns-3, SimGrid, CORE, Click)
Teaching and laboratory practice	Organizing and lecturing courses in **computer networks and system administration**, **parallel and distributed computing**, and **web development**; leading the writing of **publicly available teaching materials** (in Croatian, 340 000+ words) at **Group for apps and services on exascale research infrastructure (GASERI)**

Auxiliary skills

Open source software porting, patching, packaging, and development: Porting software to and packaging for Linux (RPM and deb) and FreeBSD (ports and pkg) using GCC and Clang compilers. Basic familiarity with porting to Windows, macOS, and illumos. Contributed patches to many open-source software projects: ns-3, Clang, LLVM, libclc, Mesa, CP2K, Sphinx, Meson Wrap DB, LaTeX Beamer class, Material for MkDocs, MoinMoin, Drogon, and Linux (kernel).

Debugging, profiling, testing, and documentation: Usage of GDB and Valgrind for debugging and profiling, including parallel and distributed applications. Test-driven development (GoogleTest and gMock). Broad experience with writing technical documentation for software development and system administration using various markup languages and tools: Markdown (MkDocs), reStructuredText (Sphinx), Doxygen, LaTeX, ConTeXt, and Pandoc; exported HTML and PDF post-processing.

Scripting languages and the Web: Experience with scripting using Python and PHP programming languages for automation of software development and system maintenance tasks as well as web application backend development. Knowledge of web application benchmarking with ApacheBench, Siege, and JMeter for scalability analysis and estimation of resource requirements for deployment.

Languages

Croatian: Native, **English**: Fluent, **Italian**: Basic, **German**: Basic

Experience

2023 – today: HPC application expert, MPCDF

Institution: *Max Planck Computing and Data Facility* (MPCDF), Max Planck Society for the Advancement of Science (MPG), Garching near Munich, Germany

Research in computational biochemistry and biophysics: Porting of the AMBER ff19SB force field to GROMACS molecular dynamics simulation software and addition of the free energy (lambda dynamics) support for per-amino-acid energy correction maps

Teaching: Seminar on Efficient Programming of HPC Systems – Frameworks and Algorithms (Advanced Seminar Course, IN2107), held by Prof. Dr. Erwin Laure (*Technische Universität München* and MPDCF)

Scientific software development: Refactoring of GROMACS code to improve developer experience, including expanding the functionality LLVM's Clang-Tidy where necessary

2019 – 2022: Co-Founder and Scientific Software Architect, RxTx Research

Startup company: RxTx Research, Rijeka, Croatia

Scientific software development: leading the development of RxDock, a fork of rDock (free and open-source molecular docking software package)

2019 – 2024: Senior Lecturer / Assistant Professor, UniRi

Institution: *Group for Applications and Services on Exascale Research Infrastructure* (GASERI), Faculty of Informatics and Digital Technologies (FIDIT), University of Rijeka, Rijeka, Croatia

Research: Distributed chemical compound database architectures; high-throughput virtual screening tools and their applications; heterogeneous system architectures and parallel algorithms; biochemical/biophysical software applications for exascale supercomputers

Teaching: Computational Biochemistry and Biophysics, Big Data Infrastructure, Code Optimization (YUFE course), Computer Networks, Security of Information and Communication Systems, Network and Mobile Operating Systems, Computer System Administration, Web Programming, Web Applications 2, Computer Networks 1, Computer Networks 2, Network Systems Management, Operating Systems 2, Distributed Systems, Parallel Programming on Heterogeneous Systems, Informatics (Biotechnology and Drug Research study program at Department of Biotechnology), Informatics for Pharmacists (Pharmacy study program at Faculty of Medicine)

Organization: Member of the University of Rijeka Supercomputing Resources Committee and Scientific Outreach Centre, Representative for Teachers in the Department Council

Promotion: Regular public lectures on popular scientific topics, presentations at European Researchers Nights, participation in open laboratory days, organization of Faculty of Informatics and Digital Technologies anniversary day celebration

2015 – 2018: Postdoctoral Researcher, HITS

Institution: *Molecular Biomechanics group* (MBM), Heidelberg Institute for Theoretical Studies (HITS), Heidelberg, Germany

Research in computational biochemistry and biophysics: Used molecular dynamics to study mechanical indentation of biological membranes and water flow around peptides

Scientific software development: Developed conditional stopping and solvent acceleration features in GROMACS, patched Mesa, Clang, LLVM, and libclc to enable running GROMACS molecular dynamics simulator via OpenCL API on AMD Radeon GPUs "out of the box" (many contributions later integrated into ROCm stack)

Computer system maintenance: Maintained group workstations, backup server, and computational biochemistry and biophysics software collection on the institute and university supercomputers; installed, configured, and maintained group-owned heterogeneous CPU/GPU computer cluster

2009 – 2019: (Senior) Research and Teaching Assistant, UniRi / RiTeh

Institution: *Computer Networks, Parallelization, and Simulation Laboratory* (CNPSLab), Department of Informatics, University of Rijeka, Rijeka, Croatia; *Department of Computer Engineering*, Faculty of Engineering (RiTeh), University of Rijeka, Rijeka, Croatia (adjunct)

Research: Optical network reliability analysis, modeling, and simulation; applications of heterogeneous computing to network routing and e-learning recommender systems; computational biochemistry, molecular modeling, and *in silico* drug design

Teaching: Computer Networks 1, Computer Networks 2 (lead the development of the online laboratory exercises for the course), Network System Management (lectures entrusted in 2018), Operating Systems 1, Operating Systems 2, Distributed Systems, Parallel Programming on Heterogeneous Systems (obtained support from NVIDIA under the CUDA Teaching Center / GPU Education Center program), Computer Networks (Computer Science study program at Faculty of Engineering)

System administration: Set up and maintained University mirror for several projects including Eclipse, cygwin, GNU, TeX Users Group / CTAN, and LibreOffice / TDF

Organization: Represented Research and Teaching Assistants in Department Council

Promotion: Regular public lectures on popular scientific topics, frequent public activities involving free and open-source software (in collaboration with Croatian Linux users group (HULK))

Education

2009 – 2015: Ph.D. in Computer Science

Institution: *Department of Telecommunications*, Faculty of Electrical Engineering and Computing (FER), University of Zagreb, Zagreb, Croatia

Focus areas: Optical telecommunication networks, communication network availability and reliability evaluation, computer network simulation and emulation

Thesis: *Method for optimizing availability of optical telecommunication network in presence of correlated failures*, supervised by Prof. Branko Mikac (retd.), defended 8th June 2015

2004 – 2009: M.Ed. in Mathematics and Informatics

Institution: *Department of Mathematics*, Faculty of Arts and Sciences (FFRi), University of Rijeka, Rijeka, Croatia

Focus areas: Real and functional analysis, mathematical foundations of quantum physics, system and network administration, free and open source software movement

Thesis: *Banach algebras*, supervised by Prof. Cvjetan Jardas (decd.), defended 17th March 2009

End of regular CV; academic CV follows.

Projects

Present projects

2023 – 2026 *BioExcel Centre of Excellence for Computational Biomolecular Research (BioExcel-3)*, led by Dr. Markus Rampp (at MPCDF), funded by Horizon Europe, EuroHPC Joint Undertaking, and also national governments of Sweden, Netherlands, Germany, Spain, Finland, and Norway

Past projects

2022 – 2023 *DPU offload of force reduction calculations in molecular dynamics simulations*, led by Dr. Vedran Miletić, funded by NVIDIA

2020 – 2022 *EuroCC – National Competence Centres in the framework of EuroHPC*, led by High-Performance Computing Center Stuttgart (HLRS), funded by Horizon 2020

2020 – 2022 *Development of Code Optimization online course for YUFE virtual campus*, led by Dr. Vedran Miletić, funded by the University of Rijeka

2019 – 2022 *Modernization, modularization, and active maintenance of RxDock*, a fast, versatile, and open-source program for docking ligands to proteins and nucleic acids, led by Dr. Vedran Miletić, funded by RxTx Research

2019 – 2021 *Biochemistry on a supercomputer: development of new software, drug-design, and analysis of disease development on molecular level*, led by Dr. Marta Žuvić, funded by the University of Rijeka, reference number uniri-prirod-18-132

2018 – 2021 *Development of the International Education Program Veleri-OI IoT School*, led by Dr. Alen Jakupović, funded by the European Social Fund

2014 – 2018 *Mechano(bio)chemistry*, led by Dr. Frauke Gräter, funded by various sources including the German Research Foundation, Heidelberg Institute for Theoretical Studies, and the University of Heidelberg

2014 – 2016 *The development and commercialization of human DNA methyltransferase Dnmt1 inhibitor with a goal to reprogram functional organization of the genome of human cells*, led by Dr. Željko Svedružić, funded by the University of Rijeka, reference number 13.11.1.2.04

2014 – 2016 *Recommender system for computer-aided learning (ELARS)*, led by Dr. Nataša Hoić-Božić, funded by the University of Rijeka, reference number 13.13.1.3.05

2014 – 2016 *RFID (Internet of Thing) based animal individual behavior intelligent identification technology and application in traceability (REMALLOY)*, led by Dr. Maja Matetić and Dr. Zetian Fu, funded by MZOS

2012 – 2014 *Establishment of CUDA Teaching Center at University of Rijeka*, led by Vedran Miletić, funded by NVIDIA

2012 – 2014 *Development of Prototype WDM Network Simulator (PWNS)*, led by Vedran Miletić, no external funding

2012 *Development of e-learning materials for Computer Networks 2 course*, led by Vedran Miletić, funded by the University of Rijeka

2008 – 2011 *Building the Future Optical Network in Europe: The e-Photon/ONe Network*, led by BONE Consortium, funded by FP7

2007 – 2013 *Supporting e-Business by Distance Learning System Based on Dialogue*, led by Dr. Božidar Kovačić, funded by MZOS

Publications

Book chapters

1. Nikolić, P., **Miletić, V.**, Odorčić, I. & Svedružić, Ž. M. In Silico Optimization of the First DNA-Independent Mechanism-Based Inhibitor of Mammalian DNA Methyltransferase DNMT1. Epi-Informatics 113–153 (2016). **doi:10.1016/B978-0-12-802808-7.00005-8**

Research papers in journals

1. Saftić Martinović, L., Birkić, N., **Miletić, V.**, Antolović, R., Štanfel, D. & Wittine, K. Antioxidant Activity, Stability in Aqueous Medium and Molecular Docking/Dynamics Study of 6-Amino- and N-Methyl-6-amino-L-ascorbic Acid. Int. J. Mol. Sci. 24(2), 1410 (2023). **doi:10.3390/ijms24021410** (WoS-SCIE, Q1 (2021), JIF: 6.208 (2021))
2. Svedružić, Ž. M, Vrbnjak, K., Martinović, M. & **Miletić, V.** Structural Analysis of the Simultaneous Activation and Inhibition of γ-Secretase Activity in the Development of Drugs for Alzheimer's Disease. Pharmaceutics 13(4), 514 (2021). **doi:10.3390/pharmaceutics13040514** (WoS-SCIE, Q1, JIF: 6.525; times cited: 3)
3. Herrera-Rodríguez, A., **Miletić, V.**, Aponte-Santamaría, C., & Gräter, F. Molecular dynamics simulations of molecules in uniform flow. Biophys. J. 116(6), 621–632 (2019). **doi:10.1016/j.bpj.2018.12.025** (WoS-SCIE, Q1, JIF: 3.854; times cited: 7)
4. Franz, F., Aponte-Santamaría, C., Daday, C., **Miletić, V.** & Gräter, F. Stability of Biological Membranes upon Mechanical Indentation. J. Phys. Chem. B 122(28), 7073–7079 (2018). **doi:10.1021/acs.jpcb.8b01861** (WoS-SCIE, Q2, JIF: 2.923; times cited: 3)
5. **Miletić, V.**, Odorčić, I., Nikolić, P. & Svedružić, Ž. M. In silico design of the first DNA-independent mechanism-based inhibitor of mammalian DNA methyltransferase Dnmt1. PLOS ONE 12(4), e0174410 (2017). **doi:10.1371/journal.pone.0174410** (WoS-SCIE, Q1, JIF: 2.766; times cited: 14)

Research papers in conference proceedings

1. **Miletić, V.**, Nikolić, P. & Kinkela, D. Structure-based Molecular Docking in the Identification of Novel Inhibitors Targeting SARS-CoV-2 Main Protease. in 2021 44th International Convention on Information, Communication, and Electronic Technology (MIPRO), 435–440 (2021). **doi:10.23919/MIPRO52101.2021.9596660**
2. **Miletić, V.**, Ašenbrener Katić, M. & Svedružić, Ž. High-throughput Virtual Screening Web Service Development for SARS-CoV-2 Drug Design. in 2020 43rd International Convention on Information, Communication, and Electronic Technology (MIPRO) 371–376 (2020). **doi:10.23919/MIPRO48935.2020.9245082**

3. **Miletić, V.**, Šubić, T. & Mikac, B. Optimizing maximum shared risk link group disjoint path algorithm using NVIDIA CUDA heterogeneous parallel programming platform. in Proceedings on the 2014 X International Symposium on Telecommunications (BIHTEL) (ed. Mrdović, S.; University of Sarajevo, Sarajevo, Bosnia and Herzegovina), 1–6 (IEEE, 2014). **doi:10.1109/BIHTEL.2014.6987645**
4. **Miletić, V.**, Holenko Dlab, M. & Hoić-Božić, N. Optimizing ELARS Algorithms Using NVIDIA CUDA Heterogeneous Parallel Programming Platform. in ICT Innovations 2014, Advances in Intelligent Systems and Computing (eds. Bogdanova, A. M. & Gjorgjevikj, D.; University of Skopje, Berlin, Heidelberg) 311, 135–144 (Springer International Publishing, 2015). **doi:10.1007/978-3-319-09879-1_14**
5. **Miletić, V.**, Maniadakis, D., Mikac, B. & Varoutas, D. On the influence of the underlying network topology on optical telecommunication network availability under shared risk link group failures. in Proceedings of the 2014 10th International Conference on the Design of Reliable Communication Networks (DRCN) (ed. Van Daele, P.; University of Ghent, Ghent, Belgium), 1–8 (IEEE, 2014). **doi:10.1109/DRCN.2014.6816135**
6. **Miletić, V.**, Mikac, B. & Džanko, M. Impact evaluation of physical length of shared risk link groups on optical network availability using Monte Carlo simulation. in Proceedings of the 2013 18th European Conference on Networks and Optical Communications (NOC) and 8th Conference on Optical Cabling & Infrastructure (OC&I) (ed. Leitgeb, E.; Technical University Graz, Graz, Austria), 249–256 (IEEE, 2013). **doi:10.1109/NOC-OCI.2013.6582897**
7. Džanko, M., Mikac, B., **Miletić, V.**, Gonzalez, N. A., Zervas, G. S. & Simeonidou, D. Analytical and simulation availability models of ROADM architectures. in Proceedings of the 12th International Conference on Telecommunications (ConTEL) (eds. Pripužić, K. & Banek, M.; University of Zagreb, Zagreb, Croatia), 39–45 (IEEE, 2013).
8. **Miletić, V.**, Mikac, B. & Džanko, M. Modelling optical network components: A network simulator-based approach. in Proceedings on the 2012 IX International Symposium on Telecommunications (BIHTEL) (ed. Mrdović, S.; University of Sarajevo, Sarajevo, Bosnia and Herzegovina), 1–6 (IEEE, 2012). **doi:10.1109/BIHTEL.2012.6412064**
9. Džanko, M., Mikac, B. & **Miletić, V.** Availability of all-optical switching fabrics used in optical cross-connects. in Proceedings on the 35th Convention International MIPRO 2012 (ed. Golubić, S.; MIPRO, Opatija, Croatia), 613–617 (IEEE, 2012).

Abstracts in conference proceedings

1. Koren, R., Martinović, M., Nikolić, P., Odorčić, I., Ostojić, L., Visentin, D., Vrbnjak, K., **Miletić, V.** & Svedružić, Ž. M. Supercomputers as microscopes for the 21st century: substrate channeling, epigenetic regulation, and molecular basis of Alzheimer's disease. in 27HSKIKI Book of Abstracts, Zagreb, Croatia (Croatian Chemical Society, 2021).
2. **Miletić, V.**, Páll, S. & Gräter, F. LLVM AMDGPU for High Performance Computing: are we competitive yet? in 2017 European LLVM Developers' Meeting, Saarbrücken, Germany (2017).
3. **Miletić, V.**, Páll, S. & Gräter, F. Towards fully open source GPU accelerated molecular dynamics simulation. in 2016 European LLVM Developers' Meeting, Barcelona, Spain (2016).
4. Nikolić, P., **Miletić, V.** & Svedružić, Ž. M. DNA Methyltransferase Dnmt1: Regulation of Substrate Selectivity. in 6th OEGMBT Annual Meeting 2014 Abstract Book (eds. Khassidov, A., Glaser, W. & Klimek, C.; Austrian Association of Molecular Life Sciences; Biotechnology; Servicebetrieb ÖH-Uni Graz GmbH, Vienna, Austria), 129 (2014).

Mentions in research paper acknowledgments

1. Turalija, M., Petrović, M. & Kovačić, B. Towards General-Purpose Long-Timescale Molecular Dynamics Simulation on Exascale Supercomputers with Data Processing Units. in 2022 45th Jubilee International Convention on Information, Communication, and Electronic Technology (MIPRO), 300–306 (2022). **doi:10.23919/MIPRO55190.2022.9803537**
2. Rennekamp, B., Kutzki, F., Obarska-Kosinska, A., Zapp, C. & Gräter, F. Hybrid Kinetic Monte Carlo/Molecular Dynamics Simulations of Bond Scissions in Proteins. *J. Chem. Theory Comput.* **16**(1), 553-563 (2020). **doi:10.1021/acs.jctc.9b00786** (WoS-SCIE, Q2, JIF: 6.006; times cited: 6)

References

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