

**CONTACT
INFORMATION**

Centre for Informatics and Computing
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**RESEARCH
INTERESTS**Parallel computing

- High-performance computing, parallel and distributed computing
- Scalability and performance portability
- Block-oriented algorithms and out-of-core programming
- Hybrid computing based on accelerators (GPU, Intel Phi)
- Algorithm optimisation

Applied mathematics

- Dense and sparse linear algebra, eigensolvers
- Macromolecular motion simulations
- Electron structure calculation

**RESEARCH
EXPERIENCE**Research Associate, Ruder Bošković Institute (10/2017 – present)

- Development of hybrid CPU-GPU BLAS-3 kernels
- High-performance out-of-core eigenvalue solvers on multi-GPU platforms
- Accelerating the simulation of complex macromolecular simulations on hybrid CPU-GPU systems
- Principal investigator on two CRO-GER bilateral projects,
- Principal investigator on the project "Scalable high-performance algorithms for future heterogeneous distributed computer systems (HybridScale)", Croatian Science Foundation, 01/2021 - 01/2026
- Participating and research scientists in more than 5 projects funded by Croatian Science Foundation, H2020, Horizon Europe programme
- Preparing project proposals for FP7, H2020, Horizon Europe, IRI and national funding.

Research Assistant, Ruder Bošković Institute (05/2009 – 10/2017)

- Development of high-performance algorithms for solving large eigenvalue problems on hybrid GPU-based platforms
- Development, design, and implementation of the out-of-core techniques and algorithms for GPUs
- Accelerating the simulation of complex macromolecular simulations on hybrid CPU-GPU systems, achieving between 2 - 5× speedup depending on the method used,
- Development and customization of cloud-based services for meteorology, bio-medicine, and digital humanities
- Coordinating the DARIAH Competence Centre (a task in the EU H2020 project *EGI-Engage*)
- Researcher on EU FP7/H2020 projects SCI-BUS, INDIGO-DataCloud, SESAME-Net
- Principal investigator on the bilateral project with RWTH Aachen on "High-performance tensor contractions on hybrid computing architectures"
- Preparing project proposals for FP7, H2020, IRI and national fundings.

Technical Associate, Ruđer Bošković Institute (05/2008 - 04/2009)

- Coordinating local activities on the two EU FP7 projects EGEE-III and SEEGRID-SCI,
- Implementing and deploying the WRF-ARW meteorological prognostic model on the SEE-GRID grid infrastructure,
- Developing a new system for easy submission and monitoring of jobs and the management of data generated by the meteorological models on the grid.

EDUCATION

Ph.D in Computer Science, 09/2008 - 10/2014

The University of Zagreb, Faculty of Electrical Engineering and Computing, Croatia

- PhD thesis title: *Solving large dense symmetric eigenproblem on hybrid architectures*
- Supervisors: Associate Professor Domagoj Jakobović, PhD and Professor Karolj Skala, PhD.D.

M.Sc. in Mathematics, 09/2003 - 04/2008

The University of Zagreb, Faculty of Science, Dept. of Mathematics, Croatia

- Master thesis title: *Acceleration of the one-sided Jacobi algorithm for finding matrix eigenvalues using sorting algorithms*
- Supervisor: Professor Sanja Singer, PhD

RESEARCH
PROJECTSRuđer Bošković Institute, Zagreb Croatia

- **Scalable high-performance algorithms for future heterogeneous distributed computer systems** Croatian Science Foundation, Installation grants 01/2021 - 01/2026
Coordinator and principal investigator. Design, development, optimization, fine-tuning and performance analysis of linear algebra algorithms on distributed heterogeneous computing systems (HPC, supercomputers). Applications of novel HPC linear algebra kernels in physics, computational chemistry and biomedicine scientific software.
- **Light on Molecules: Exploration of Coupled Electron and Nuclear Dynamics** Croatian Science Foundation (03/2017 - 03/2021)
Optimisation and acceleration of nonadiabatic molecular simulations on hybrid GPU-based systems.
- **High-performance tensor contractions on hybrid computing architectures** CRO-GER bilateral project between RWTH Aachen, Ruđer Bošković Institute and Faculty of Mechanical Engineering and Naval Architecture The University of Zagreb, funded by the Ministry of Science, Education and Sports of the Republic of Croatia (01/2017 - 12/2019)
Project leader. Improving performance portability and scalability of FLEUR code (electron structure calculation code) using multi-GPU and multi-CPU systems. Design and implementation of full hybrid BLAS-3 kernels.
- **INDIGO-DataCloud – INtegrating Distributed data Infrastructures for Global Exploitation**
H2020 Framework Programme, European Commission, 04/2015 - 09/2017
Developing a Repository-as-a-Service based on the Invenio repository framework in the European Open Cloud space for Digital Arts and Humanities researchers and scholars
- **SESAME-NET – Supercomputing Expertise for Small and Medium Enterprise Network**
H2020 Framework Programme, European Commission, 06/2015 - 05/2017

Promoting HPC technologies and establishing a network of HPC centres in the region to support small and medium enterprises.

- **EGI-Engage – Engaging the EGI Community towards an Open Science Commons**

H2020 Framework Programme, European Commission, *03/2015 - 08/2017*

Task leader. Coordinating the establishment of the DARIAH Competence Centre. Maintaining cloud-based services for DARIAH (Digital Humanities) research community

- **COST Action IC1305 - Network for Sustainable Ultrascale Computing (NESUS)**

COST Programme, European Commission, *03/2014 - 03/2018*

Management committee deputy. Participating in the work of two Working groups "Applications" and "Programming models and runtimes". Designing and developing dense linear algebra routines (full/partial eigenvalue spectrum), improve the energy consumption of the conjugate gradient method on GPU accelerators.

- **Scalable Big Data Bioinformatics Analysis in the Cloud**

CRO-AUT bilateral project with Medical University of Innsbruck, Austria, funded by Ministry of Science, Education and Sports of the Republic of Croatia (*01/2014 - 12/2016*)

Implementing an automatic deployment and configuration of the Hadoop cluster in the Amazon EC2 cloud environment using the CloudMan cloud manager framework.

- **SCI-BUS: Scientific gateway Based User Support**

7th Framework Programme (FP7), European Commission (*09/2012 - 09/2014*)

Establishing and maintaining the Adria Science Gateway for setting, executing and managing workflow-based weather prediction forecasting simulations (WRF prognostic model) in various distributed environments (cluster, grid and cloud).

- **Optimization of energy consumption in distributed computing systems**

CRO-SLO bilateral project with Jozef Stefan Institute, Ljubljana, Slovenia, funded by Ministry of Science, Education and Sports of the Republic of Croatia (*01/2012 - 12/2013*)

Analyzing and testing the impact of thread binding on the overall energy consumption of existing applications.

- **COST Action IC0805 - Open Network for High-Performance Computing on Complex Environments (ComplexHPC)**

COST Programme, European Commission, *04/2012 - 07/2013*

Researching and developing novel out-of-core algorithms for solving large eigenvalue problems on non-distributed (shared) memory systems equipped with GPU accelerators.

- **SEEGRD-SCI – SEE-GRID eInfrastructure for regional eScience**

7th Framework Programme (FP7), European Commission (*05/2008 - 04/2010*)

Porting and performance testing of the Weather Research and Forecasting (WRF) model on the South European grid infrastructure.

- **EGEE-III – Enabling Grids for eScience**

7th Framework Programme (FP7), European Commission (*05/2008 - 04/2010*)

Porting and performance testing of the Weather Research and Forecasting model on European grid infrastructure (EGI).

- 2015 Best paper award, event *38th International Convention on Information and Communication Technology, Electronics and Microelectronics*, Opatija, Croatia. Paper title: *"Cloudflow - A Framework for MapReduce Pipeline Development in Biomedical Research"*. Authors: Lukas Forer, Enis Afgan, Hansi Weißensteiner, **Davor Davidović**, Günter Specht, Florian Kronenberg, Sebastian Schönherr.
- 2014 Silver Plaque "Josip Lončar" for the PhD thesis *"Solving large dense symmetric eigenproblem on hybrid architectures."*, an annual award by the Faculty of Electrical Engineering and Computing, The University of Zagreb, to doctoral students in recognition of outstanding doctoral dissertations.
- 2003-2008 State Student Scholarship awarded by the Ministry of Science, Education and Sports of the Republic of Croatia.

PROFESSIONAL
TRAINING

Summer schools and workshops

Summer School: *Workflows and Gateways for Grids and Clouds*

- Duration: 1st - 6th July, 2013
- Venue: the Computer and Automation Research Institute, Hungarian Academy of Sciences, Budapest, Hungary

Summer School: *Heterogeneous computing - impact on algorithms*

- Duration: 3rd - 7th June, 2013
- Venue: Uppsala University, Uppsala, Sweden

Workshop: *WS-PGRADE/gUSER Code Camp*

- Duration: 28th - 30th November, 2012
- Venue: the Computer and Automation Research Institute, Hungarian Academy of Sciences, Budapest, Hungary

Short research visits

- **Barcelona Supercomputing Center, Barcelona, Spain, HPC-Europa3 Transnational Access programme (01/04/2019 - 28/04/2019)**
Design, implementation, fine-tuning and performance analysis of the task-based left-looking LU factorization with block pivoting on shared-memory systems.
- **University Jaume I, Castellón de la Plana, Spain, COST Action IC1305 (24/01/2015 - 08/02/2015)**
Reduce execution time and improve the energy consumption of the Conjugate Gradient (CG) method for the iterative solution of sparse linear systems using the Dynamic Parallelism feature of NVIDIA GPU devices.
- **University Jaume I, Castellón de la Plana, Spain, COST Action IC0805 (21/09/2012 - 16/10/2012)**
Design and development of the spectral divide-and-conquer QDWH-based algorithm for large symmetric eigenproblems on GPU. Design of the novel left-looking, memory-efficient QR factorization on GPUs for structured matrices.
- **University Jaume I, Castellón de la Plana, Spain (02/2011 - 07/2011)**
Development and implementation of the multi-stage and the Krylov-subspace based eigenvalue solvers for dense symmetric eigenproblems. The development of the algorithms that exhibit very high performances on a GPU even when storage space exceeds the GPU memory (out-of-core execution with the respect to

the GPU memory). Optimization of data transfers between the main memory and the GPU memory. Design and implementation of the high-performance scalable algorithms on hybrid CPU-GPU computing architectures.

- **Summer internship in ETH Zurich, Switzerland (08/2009)**

Work on the implementation and speedup of the Hessenberg reduction on hybrid CPU-GPU system using NVIDIA CUDA programming model.

TECHNICAL SKILLS

- **Operating systems:** Unix/Linux, Windows
- **Development environments:** Eclipse, Netbeans, PyCharm, Nsight
- **Programming Languages:** C/C++, Python, Java, Fortran
- **Mathematical and statistical computing:** Matlab, Mathematica, Octave, Numpy
- **Computational libraries:** CUBLAS, CUBLASxt, MAGMA, LAPACK, BLAS, ScaLAPACK, MKL
- **Parallelization models:** MPI, OpenMP, CUDA
- **Virtualization technologies:** Docker, Amazon AWS, VMware, VirtualBox

ORGANIZATIONAL SKILLS

Perennial teamwork experience acquired by working in an international team within EU projects

Project leadership experience gained during the EGI-Engage project (task leader) and the bilateral CRO-GER project (coordinator)

SOCIAL SKILLS

Communicative
Easily approachable

HOBBIES

Mounting hiking
Travelling

SELECTED PUBLICATIONS

Journal papers

- [1] Alonso-Jordá, P., Davidović, D., Sapunar, M., Herrero, J., Quintana-Ortí, E. (2021) Efficient update of determinants for many-electron wave function overlaps. *Computer physics communications*, 258, 107521, 14 doi:10.1016/j.cpc.2020.107521.
- [2] Sapunar, M., Piteša, T., Davidović, D., Došlić, N. (2019) Highly Efficient Algorithms for CIS Type Excited State Wave Function Overlaps. *Journal of chemical theory and computation*, 15 (6), 3461-3469 doi:10.1021/acs.jctc.9b00235.
- [3] Aliaga, J., Alonso, P., Badía, J., Chacón, P., Davidović, D., López-Blanco, J., Quintana-Ortí, E. (2016) Fast Band-Krylov Eigensolver for Macromolecular Functional Motion Simulation on Multicore Architectures and Graphics Processors. *Journal of computational physics*, 309, 314-323 doi:10.1016/j.jcp.2016.01.007.
- [4] Aliaga, J., Bientinesi, P., Davidović, D., Di Napoli, E., Igual Peña, F., Quintana-Ortí, E. (2012) Solving Dense Generalized Eigenproblems on Multi-threaded Architectures. *Applied mathematics and computation*, 218 (22), 11279-11289 doi:10.1016/j.amc.2012.05.020.

- [5] Singer, S., Singer, S., Novaković, V., Davidović, D., Bokulić, K., Ušćumlić, A. (2012) Three-Level Parallel J-Jacobi Algorithms for Hermitian Matrices. *Applied mathematics and computation*, 218 (9), 5704-5725 doi:10.1016/j.amc.2011.11.067.

Conference papers

- [6] Mijić, N., Davidović, D. (2022) Batched matrix operations on distributed GPUs with application in theoretical physics. U: *Proceedings of 45th Jubilee International Convention on Information, Communication and Electronic Technology (MIPRO)* doi:10.23919/mipro55190.2022.9803591.
- [7] Wu, X., Davidović, D., Achilles, S., Di Napoli, E. (2022) ChASE: a distributed hybrid CPU-GPU eigensolver for large-scale hermitian eigenvalue problems. U: *PASC'22: Proceedings of the Platform for Advanced Scientific Computing Conference* doi:10.1145/3539781.3539792.
- [8] Davidović, D., Quintana-Ortí, E. (2020) Structure-Aware Calculation of Many-Electron Wave Function Overlaps on Multicore Processors. U: *Wyrzykowski, R., Deelman, E., Dongarra, J., Karczewski, K. (ur.) LNCS 12043: Parallel Processing and Applied Mathematics* doi:10.1007/978-3-030-43229-4_2.
- [9] Aliaga, J., Davidović, D., Pérez, J., Quintana-Ortí, E. (2016) Harnessing CUDA Dynamic Parallelism for the Solution of Sparse Linear Systems. U: *Joubert, G.R., Leather, H., Parsons, M., Peters, F., Sawyer, M. (ur.) Advances in Parallel Computing Volume 27: Parallel Computing: On the Road to Exascale.* (<https://www.bib.irb.hr/815878>).
- [10] Aliaga, J., Davidović, D., Quintana-Ortí, E. (2014) Out-of-core solution of eigenproblems for macromolecular simulations. U: *Wyrzykowski, R., Dongarra, J., Karczewski, K., Waśniewski, J. (ur.) Parallel Processing and Applied Mathematics, Lecture Notes in Computer Science, Vol. 8384.*
- [11] Davidović, D., Enrique S. Quintana-Ortí (2012) Applying OOC Techniques in the Reduction to Condensed Form for Very Large Symmetric Eigenproblems on GPUs. U: *Rainer Stotzka, Michael Schiffers, and Yiannis Cotronis (ur.) Euromicro Conference on Parallel, Distributed and Network-based Processing.*

Full list of publications

Croatian Scientific Bibliography:

<https://www.bib.irb.hr/pregled/znanstvenici/315432>