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CONTACT INFORMATION	Centre for Informatics and Computing Ruder Bošković Institute Bijenička cesta 54 10 000 Zagreb, Croatia	<i>Mobile:</i> +385 98 9611 483 <i>Office:</i> +385 1 456 1091 <i>E-mail:</i> ddavid@irb.hr
RESEARCH INTERESTS	<u>Parallel computing</u> <ul style="list-style-type: none"><li>• Dense and sparse linear algebra</li><li>• Scalability and performance portability</li><li>• Block-oriented algorithms and out-of-core programming</li><li>• Hybrid computing based on GPU accelerators</li></ul> <u>Applied mathematics</u> <ul style="list-style-type: none"><li>• Dense and sparse linear algebra, eigensolvers</li><li>• Macromolecular motion simulations</li><li>• Electron structure calculation</li></ul>	
RESEARCH EXPERIENCE	<u>Research Associate, Ruder Bošković Institute (10/2017 – present)</u> <ul style="list-style-type: none"><li>• Development of hybrid CPU-GPU BLAS-3 kernels,</li><li>• High-performance out-of-core eigenvalue solvers on multi-GPU platforms,</li><li>• Accelerating the simulation of complex macromolecular simulations on hybrid CPU-GPU systems,</li><li>• Principal investigator on two bilateral project with Germany,</li><li>• Croatian NSF project "LightMol", design and implementation of specialized kernels for computing nonadiabatic molecular dynamic simulations on GPUs,</li><li>• Researcher on two H2020 projects (EOSC-Hub and NI4OS).</li><li>• Preparing project proposals for FP7, H2020, IRI and national fundings.</li></ul> <u>Research Assistant, Ruder Bošković Institute (05/2009 – 10/2017)</u> <ul style="list-style-type: none"><li>• Development of high-performance algorithms for solving large eigenvalue problems on hybrid GPU-based platforms</li><li>• Development, design, and implementation of the out-of-core techniques and algorithms for GPUs</li><li>• Accelerating the simulation of complex macromolecular simulations on hybrid CPU-GPU systems, achieving between 2 - 5× speedup depending on the method used,</li><li>• Development and customization of cloud-based services for meteorology, biomedicine, and digital humanities</li><li>• Coordinating the DARIAH Competence Centre (a task in the EU H2020 project <i>EGI-Engage</i>)</li><li>• Researcher on EU FP7/H2020 projects SCI-BUS, INDIGO-DataCloud, SESAME-Net</li><li>• Principal investigator on bilateral project with RWTH Aachen on "High performance tensor contractions on hybrid computing architectures"</li><li>• Preparing project proposals for FP7, H2020, IRI and national fundings.</li></ul> <u>Technical Associate, Ruder Bošković Institute (05/2008 - 04/2009)</u> <ul style="list-style-type: none"><li>• Coordinating local activities on the two EU FP7 projects EGEE-III and SEEGRID-SCI,</li></ul>	

- 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

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, Ph.D. and Professor Karolj Skala, Ph.D.

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

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, Ph.D.

## RESEARCH PROJECTS

Ruder Bošković Institute, Zagreb Croatia

- **Optimization of Material Science algorithms on hybrid HPC platforms**  
CRO-GER bilateral project between Juelich Supercomputing centre, Ruder Bošković Institute and Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, funded by Ministry of Science, Education and Sports of the Republic of Croatia (01/2019 - 12/2020)  
Project leader. Design and development of the ChASE library for hybrid multi-GPU/multi-CPU platforms. Optimization and implementation of the library's functions in C/C++/CUDA.
- **EOSC-hub – Integrating and managing services for the European Open Science Cloud**  
H2020 Framework Programme, European Commission, 01/2018 - 12/2020  
Integration of the DARIAH science gateway and applications with EOSC tools (cloud, accounting, hosting, authentication, marketplace), service maintenance, organizing training event and dissemination of the project's outcomes.
- **Light on Molecules: Exploration of Coupled Electron and Nuclear Dynamics**  
Croatian Science Foundation (03/2017 - present)  
Optimization 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, Ruder Bošković Institute and Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, funded by Ministry of Science, Education and Sports of the Republic of Croatia (01/2017 - 12/2017)  
Project leader. Improving performance portability and scalability of FLEUR code (electron structure calculation code) using multi-GPU and multi-CPU systems. Design and implementation 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 energy consumption of conjugate gradient method on GPU accelerators.
- **Scalable Big Data Bioinformatics Analysis in the Cloud**  
CRO-ATU 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 Hadoop cluster in the Amazon EC2 cloud environment using 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 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 Infrastructure 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).

AWARDS	<p>2015 Best paper award, event <i>38th International Convention on Information and Communication Technology, Electronics and Microelectronics</i>, Opatija, Croatia. Paper title: "<i>Cloudflow - A Framework for MapReduce Pipeline Development in Biomedical Research</i>". Authors: Lukas Forer, Enis Afgan, Hansi Weißensteiner, <b>Davor Davidović</b>, Günter Specht, Florian Kronenberg, Sebastian Schönherr.</p> <p>2014 Silver Plaque "Josip Lončar" for the PhD thesis "<i>Solving large dense symmetric eigenproblem on hybrid architectures.</i>", annual award by Faculty of Electrical Engineering and Computing, University of Zagreb to doctoral students in recognition of outstanding doctoral dissertations.</p> <p>2003-2008 State Student Scholarship awarded by the Ministry of Science, Education and Sports of the Republic of Croatia.</p>
PROFESSIONAL TRAINING	<p><u>Summer schools and workshops</u></p> <p><b>Summer School: <i>Workflows and Gateways for Grids and Clouds</i></b></p> <ul style="list-style-type: none"> <li>• Duration: 1<sup>st</sup> - 6<sup>th</sup> July, 2013</li> <li>• Venue: the Computer and Automation Research Institute, Hungarian Academy of Sciences, Budapest, Hungary</li> </ul> <p><b>Summer School: <i>Heterogeneous computing - impact on algorithms</i></b></p> <ul style="list-style-type: none"> <li>• Duration: 3<sup>rd</sup> - 7<sup>th</sup> June, 2013</li> <li>• Venue: Uppsala University, Uppsala, Sweden</li> </ul> <p><b>Workshop: <i>WS-PGRADE/gUSER Code Camp</i></b></p> <ul style="list-style-type: none"> <li>• Duration: 28<sup>th</sup> - 30<sup>th</sup> November, 2012</li> <li>• Venue: the Computer and Automation Research Institute, Hungarian Academy of Sciences, Budapest, Hungary</li> </ul> <p><u>Short scientific visits</u></p> <p><b>Research Visit - HPC-Europa3</b></p> <ul style="list-style-type: none"> <li>• Duration: 1<sup>st</sup> April - 27<sup>th</sup> April 2019</li> <li>• Venue: Barcelona Supercomputing Centre, Barcelona, Spain</li> <li>• Host: Pedro Valero Lara, PhD</li> <li>• Activities: <ul style="list-style-type: none"> <li>Design and implementation of a look-ahead variant of the partial pivoting LU factorization using the OmpSs task-based programming model for multi-core platforms.</li> <li>Testing and validation on the algorithm on the BSC supercomputer (CTE-POWER)</li> </ul> </li> </ul> <p><b>Short-Term Scientific Mission - COST Action IC1305</b></p> <ul style="list-style-type: none"> <li>• Duration: 24<sup>th</sup> January - 8<sup>th</sup> February 2015</li> <li>• Venue: University Jaume I, Castellón de la Plana, Spain</li> <li>• Host: Prof. Enrique S. Quintana-Ortí</li> <li>• Activities: <ul style="list-style-type: none"> <li>Reduce execution time and improve energy consumption of the Conjugate Gradient (CG) method for the iterative solution of sparse linear systems using Dynamic Parallelism feature of NVIDIA GPU devices.</li> </ul> </li> </ul> <p><b>Short-Term Scientific Mission - COST Action IC0805</b></p> <ul style="list-style-type: none"> <li>• Duration: 21<sup>st</sup> September - 16<sup>th</sup> October 2012</li> <li>• Venue: University Jaume I, Castellón de la Plana, Spain</li> <li>• Host: Prof. Enrique S. Quintana-Ortí</li> </ul>

- **Activities:**  
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.

#### **Research visit University Jaume I**

- Duration: February - July, 2011
- Venue: University Jaume I, Castellón de la Plana, Spain
- Host: Prof. Enrique S. Quintana-Ortí
- **Activities:**  
Development and implementation of the multi-stage and the Krylov-subspace based eigenvalue solvers for dense symmetric eigenproblems. The development of the algorithms that exhibits 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 and the GPU memory. Design and implementation of the high-performance scalable algorithms on hybrid CPU-GPU computing architectures.

#### **Summer internship in ETH Zurich**

- Duration: 1<sup>st</sup> - 31<sup>st</sup> August 2008
- Venue: ETH, Zurich, Switzerland
- Host: Prof. Daniel Kressner
- **Activities:**  
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
- **Programming Languages:** C/C++, Python, Java, Fortran
- **Mathematical and statistical computing:** Matlab, Mathematica, Octave
- **Computational libraries:** CUBLAS, CUBLASxt, MAGMA, LAPACK, BLAS, ScaLAPACK, MKL
- **Parallelization models:** MPI, OpenMP, CUDA, OmpSs
- Virtualization technologies: Docker, Amazon AWS

#### ORGANIZATIONAL SKILLS

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

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

#### SOCIAL SKILLS

Communicative  
Easily approachable

#### HOBBIES

Mounting hiking  
Travelling

#### SELECTED PUBLICATIONS

#### **Journal papers**

- [1] Sapunar, Marin; Piteša, Tomislav; **Davidović, Davor**; Došlić, Nada. Highly Efficient Algorithms for CIS Type Excited State Wave Function Overlaps. *Journal of Chemical Theory and Computation*. (2019) (accepted for publication)
- [2] **Davidovic, Davor**; Fabregat-Traver, Diego; Höhnerbach, Markus; Di Napoli, Edoardo. Accelerating the computation of FLAPW methods on heterogeneous architectures. *Concurrency Computat Pract Experience*, 30(2018), 24; e4905, doi:10.1002/cpe.4905
- [3] Aliaga, José I.; Alonso, Pedro; Badía, José M.; Chacón, Pablo; **Davidović, Davor**; López-Blanco, José R.; Quintana-Ortí, Enrique S. Fast Band–Krylov Eigensolver for Macromolecular Functional Motion Simulation on Multicore Architectures and Graphics Processors. *Journal of computational physics*, 309 (2016); 314-323
- [4] Forer, Lukas; Afgan, Enis; Weißenteiner, Hansi; **Davidović, Davor**; Specht, Guenther; Kronenberg, Florian; Schöenherr, Sebastian. CLOUDFLOW - Enabling Faster Biomedical Pipelines with Mapreduce and Spark. *Scalable Computing: Practice and Experience*, 17 (2) (2016); 103-114
- [5] Aliaga, José I.; Badia, Jose M.; Castillo, Maribel; **Davidović, Davor**; Mayo, Rafael; Quintana-Ortí, Enrique S. Out-of-core macromolecular simulations on multi-threaded architectures. *Concurrency and Computation: Practice and Experience*, 27 (6) (2015); 1540-1550
- [6] Aliaga, José I.; Bientinesi, Paolo; **Davidović, Davor**; Di Napoli, Eduardo; Igual Peña, Francisco D.; Quintana-Ortí, Enrique S. Solving Dense Generalized Eigenproblems on Multi-threaded Architectures. *Applied Mathematics and Computation*, 218 (22) (2012); 11279-11289
- [7] Singer, Sanja; Singer, Saša; Novaković, Vedran; **Davidović, Davor**; Bokulić, Krešimir; Ušćumlić, Aleksandar. Three-Level Parallel J-Jacobi Algorithms for Hermitian Matrices. *Applied Mathematics and Computation*, 218 (9) (2012); 5704-5725

#### Conference papers

- [8] Fabregat-Traver, Diego; **Davidović, Davor**; Höhnerbach, Markus; Di Napoli, Edoardo. Hybrid CPU-GPU generation of the Hamiltonian and Overlap matrices in FLAPW methods. *LNCS - High Performance Scientific Computing*, Springer (2017); 200-211
- [9] Aliaga, José; **Davidović, Davor**; Pérez, Joaquín; Quintana-Ortí, Enrique S. Harnessing CUDA dynamic parallelism for the solution of sparse linear systems. In: *International Conference on Parallel Computing (PARCO) Advances in Parallel Computing: Parallel Computing: On the Road to Exascale*, Vol. 27, IOS Press (2016);. 217-226
- [10] Aliaga, José I.; **Davidović, Davor**; Quintana-Ortí, Enrique S. Out-of-core solution of eigenproblems for macromolecular simulations. *Parallel Processing and Applied Mathematics, Lecture Notes in Computer Science*, Vol. 8384, Springer (2014); 490-499
- [11] **Davidović, Davor**; Enrique S. Quintana-Ortí. Applying OOC Techniques in the Reduction to Condensed Form for Very Large Symmetric Eigenproblems on GPUs. *Euromicro Conference on Parallel, Distributed and Network-based Processing*, IEEE Computer Society CPS (2012); 442-449

- [12] Afgan, Enis; Skala, Karolj; **Davidović, Davor**; Lipić, Tomislav; Sović, Ivan. Cloud-Man as a tool execution framework for the cloud. MIPRO 2012: Proceedings of the 35th International Convention Convention on Information and Communication Technology, Electronics and Microelectronics, 2012, Rijeka, Croatia.

**Full list of publications**

Croatian Scientific Bibliography:

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