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Životopis:

Dušan Račko študoval čiastočne na Ústave polymérov Slovenskej akadémie vied a čiastočne na Katedre chémie Florentskej univerzity a v Európskom laboratóriu pre nelineárnu spektroskópiu vo Florencii, kde pracoval v skupine Molecular spectroscopy & simulations. prof. Gianniho Cardiniho v rokoch 2000 až 2005. Témou jeho dizertačnej práce boli počítačové simulácie kondenzovaných molekulárnych fáz.

Neskôr sa šiel na postdoktorandskú stáž do Španielska, kde od septembra 2007 do septembra 2010 strávil tri roky čiastočne na Chemickej fakulte Baskickej univerzity a čiastočne v Donostia International Physics Center, kde pracoval na počítačových simuláciách molekulovej dynamiky polymérnych tavenín v skupine Polymers & Soft Matter Prof. Juana Colmenera de León.

Po návrate na Ústav Polymérov Slovenskej Akadémie Vied v roku 2010 nastúpil ako samostatný vedecký pracovník do Oddelenia Molekuláových Simulácií Polymérov v skupine Prof. Petra Cifru, kde sa venuje počítačovým simuláciám molekulovej dynamiky biopolymérov DNA a komplexných molekulárnych systémov.

Dušan Račko neskôr od augusta 2014 do júla 2018 strávil štyri roky na expertnom pobyte vo Švajčiarsku v Centre integratívnej genomiky, ktoré je súčasťou Fakulty biológie a medicíny Univerzity v Lausanne, v skupine Modelovania chromatínu a DNA Prof. Andrzeja Stasiaka, kde sa zaoberal počítačovými simuláciami DNA, študujúc aspekty topológie DNA a molekulárnej biológie. V januári 2015 sa skupina stala aj súčasťou Švajčiarskeho inštitútu bioinformatiky.

Po návrate na Ústav polymérov SAV sa stal od júna 2019 vedúcim Oddelenia Molekulových Simulácií Polymérov.

Dušan Račko je autorom asi 35 publikácií CC s asi 650 citáciami. Prezentoval alebo sa zúčastnil na približne 130 konferenčných príspevkoch, vrátane približne 30 prednášok v EÚ a USA. Doposiaľ dostal 5 (plne hradených) pozvaní prednášať o svojich prácach o počítačových simuláciách na medzinárodných fórach po celom svete.

Dušan Račko okrem vedeckej činnosti žil aj dva roky v Maroku. Hovorí francúzsky a anglicky, trochu španielsky, taliansky a rusky. Má rád výpočtovú techniku, populárnu vedu a cestovanie. Okrem iného navštívil CERN v Ženeve, stavenisko prvej svetovej fúznej elektrárne (ITER) v Cadarache, najstaršiu univerzitu na svete v Bologni,

najvýkonnejší európsky superpočítač v stredisku High Performance Computing Center v Stuttgarte, atď.

Vedecké záujmy:

computer simulations, molecular simulations, DNA, DNA topology, DNA and condensed matter, polymers and material modeling

Zamestnanie:

2019 - Head of Department of Molecular Simulations of Polymers, Polymer Institute, Slovak Academy of Sciences, Department of Molecular Simulations of Polymers, Bratislava, Slovakia

2015 - 2018 Research Associate, Swiss Institute of Bioinformatics, DNA and Chromosome Modeling group, Lausanne, Switzerland

2014 - 2018 Premier Assistant, University of Lausanne, Faculty of Biology and Medicine, Center for Integrative Genomics (CIG), DNA and Chromosome Modeling group, Lausanne, Switzerland

2010 - 2017 Associate Professor, Polymer Institute, Slovak Academy of Sciences, Department of Molecular Simulations of Polymers, Bratislava, Slovakia

2007 - 2010 post-doc, Donostia International Physics Center, Polymers & soft matter group, Donostia-San Sebastián, Spain

2007 - 2010 post-doc, Universidad del País Vasco / Euskal Herriko Unibertsitatea, Department of Chemistry, Polymers & soft matter group, Donostia-San Sebastián, Spain

2003 - 2004 PhD Fellow (Marie-Curie Training Fellowship), University of Florence, Dipartimento di Chimica "Ugo Schiff", Molecular spectroscopy & simulations group, Florence, Italy

2003 - 2004 PhD Fellow (Marie-Curie Training Fellowship), European Laboratory for Non-Linear Spectroscopy, Molecular spectroscopy & simulations group, Florence, Italy

Spolupráce:

2023 - University of Trento, Dr. Luca Tubiana
2022 - University of Edinbourgh, Dr. Davide Michieletto
2020- University of Vienna, bilateral project on topological glasses with Dr. Jan Smrek
2019-2020 University of Adelaide, Faculty of Sciences, School of Biological Sciences, collaboration with Dr. Ian Dodd on modelling of gene expression by using coarse grained simulations of bacterial DNA
2019- Informal collaboration with Prof. Andrzej Stasiak (formalized e.g. in EUTOPIA STSM and acknowledged in papers)

2018-2020 GA Drilling Co., Contracted collaboration as external expert on consulting chemistry, engineering and usage of oil based muds and bio-fuels during design, performance and safety of drilling equipment
2018- Institute of Physics of the Slovak Academy of Sciences – molecular simulations of confined molecules and comparison with experimental free volume
2010-2012 Department of Composite Materials at Polymer Institute of the Slovak Academy of Sciences, a collaboration with Prof. Igor Krupa formalized within EP7 NOMS project on modelling and design of a nano-mechanical photoactuating device
2000-2003 International Laser Center, Ilkovičova 2961/3, 841 04 Karlova Ves, Bratislava, Slovakia: Informal collaboration on atomistic molecular simulations with Prof Dusan Chrovat

Vzdelanie:

02.12.2011 **Samostatný vedecký pracovník** – vedecký kvalifikačný stupeň IIa

2000 – 2005 Doctor of Philosophy, Polymer Institute of the Slovak Academy of Sciences, in Bratislava, Slovakia

1995 – 2000 Engineer's title, Faculty of Chemical and Food Technology, Department of Chemical Engineering, Slovak University of Technology, Bratislava, Slovakia

Pozvané prednášky:

[5] **D. Račko:** „Molecular Simulations of DNA Topology", Department of Physics, University of Trento, Italy, 19 – 25 March 2023

[4] **D. Račko et al.:** "Generation of supercoils in nicked and gapped DNA drives DNA unknotting and postreplicative decatenation", Workshop on Knots and Links in Biological and Soft Matter Systems, 19 -24 September 2016, Trieste, Italy.

[3] **D. Račko:** "What can we learn from various free volume properties as obtained from computer simulations of polymer condensed phases", 24-27. May 2011, Mainz Materials Simulations Days 2011, Mainz, Germany.

[2] **D. Račko:** "The Free Volume of PVME as Computed in a Range of Temperatures and Length Scales up to the nano Region", 39th Seminar on the Positron Annihilation, PSPA10, 20-25 June 2010, Kazimiers, Poland.

[1] **D. Račko:** "Molecular simulations of polymers with case studies" International Summer school on Polymers, Congress Center of the Slovak Academy of Sciences, 22-26 August 2011, Smolenice, Slovakia.

Členstvá a ocenenia

Memberships:
(2022) Member of Electorial Board for Director of PI SAS (2021 -) Member of Management Board of the Polymer Institute SAS (June 2019-) Head of Department of Molecular Simulations of Polymers at Polymer Institute SAS. (2020-) Member of

Scientific Committee XI. Slovak-Czech Conference on Polymers "Polyméry 2020", (2020-) Board for External Communication with Industry, (2019-) Supervising a PhD Thesis "Chromosome and DNA modeling", (2019) Committee member for PhD students, (2019) A Guest Editor in MDPI Computation, (2019) A member of organizing committee BIMac2019, (2017) Review editor in Frontiers in Molecular Biophysics, Frontiers in Physics, (2016) Guest editor in MDPI Polymers, (2014-2018) Member of Scientific board of Polymer Institute of the Slovak Academy of Sciences, (2011) Member of organizing committee of the 10 th International Workshop on Positron and Positronium Chemistry, (2011) Member of Scientific board at the International Summer School on polymers in Smolenice, (2011-) Member of the Slovak Physical Society

Ocenenia:
(2021) Prize of the Slovak Academy of Sciences for achievements in science and research, June 29 (2021) 1st place poster prize at "Interdisciplinary Challenges in Nonequilibrium Physics" Erwin Schroedinger Institute April 12-16 (2013) 2nd place poster award, at the EUROFILLERS 2014 conference, August 25-29, 2013, (2011) Best Young Scientist Paper Award at Polymer Institute in 2011, (2011) Certificate of Honor – award by Presidium of the Slovak Academy of Sciences for collection of works for a scientist under 35 years of age (2005), FP5 Marie Currie Training Fellowship

Publikácie (WOS):

[36] R. Ruskova, **D. Racko*** "Pushing polymers through chiral channels" (in preparation)

[35] R. Ruskova, L. Tubiana, R. Pottestio, **D. Racko*** "Controlling composite knots with chiral channels" (in preparation)

[34] R. Ruskova, **D. Racko***, "Knot Factories with Helical Geometry Enhance Knotting and Induce Handedness to Knots" Polymers 2022, 14(19), 4201; https://doi.org/10.3390/polym14194201

[33] R. Ruskova, **D. Racko*** "Channels with Helical Modulation Display Stereospecific Sensitivity for Chiral Superstructures" Polymers, 2021, 13(21), 3726; https://doi.org/10.3390/polym13213726

[32] R. Ruskova, **D. Racko*** "Entropic competition between supercoiled and torsionally relaxed chromatin fibres drives loop extrusion through pseudo-topologically bound cohesin." Biology 2021, 10(2), 130

[31] S. Capponi, F. Alvarez, **D. Racko*** "Free volume in PVME-Water Solution" Macromolecules 2020, 53, 12, 4770–4782.

[30] **D. Racko**, F. Benedetti, J. Dorier, A. Stasiak "Are TAD's Supercoiled?" Nucleic Acids Res. 47, 521-532 (2019)

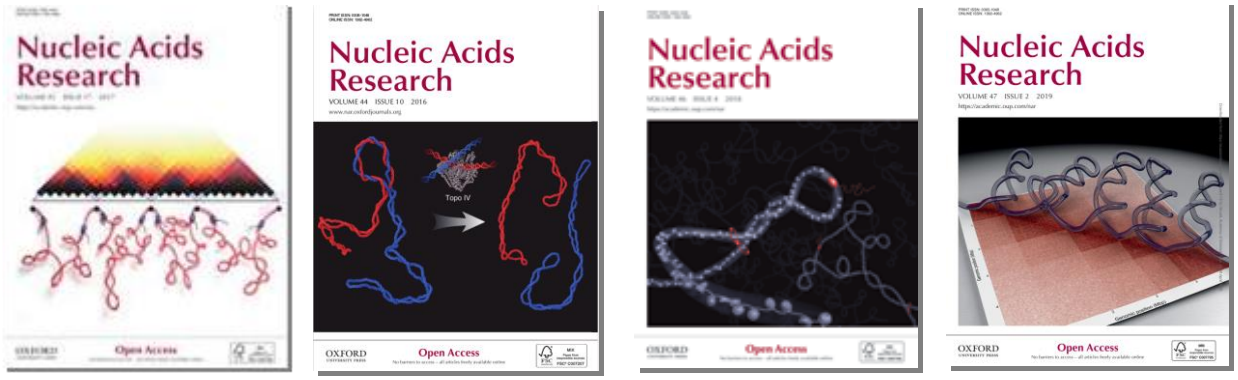
[29] **D. Racko**, F. Benedetti, J. Dorier, A. Stasiak "Chromatin Loop Extrusion and Chromatin Unknotting" Polymer 10 (2018)

[28] F. Benedetti, **D. Racko**, J. Dorier, A. Stasiak, “Introducing supercoiling into models of chromosome structure” Modelling 3D Conformation of Genome, edited by G. Tiana and L. Giorgetti, Series in Computational Biophysics, invited chapter 2018.

[27] **Racko D**, Benedetti F, Dorier J, Stasiak A. “Transcription-induced supercoiling as the driving force of chromatin loop extrusion during formation of TADs in interphase chromosomes”, Nucleic Acids Res 46(4) 1648-1660 (2018)

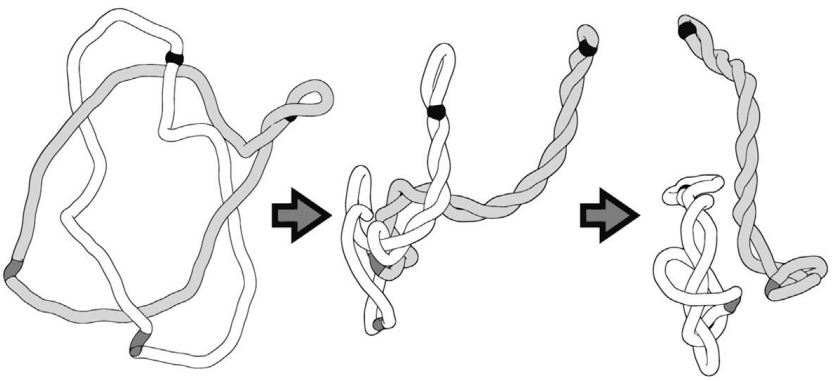
[26] Benedetti F, **Racko D**, Dorier J, Burnier Y, Stasiak A: "Transcription-induced supercoiling explains formation of self-interacting chromatin domains in S. pombe" Nucleic Acids Res., 15, (2017) https://academic.oup.com/nar/article-abstract/doi/10.1093/nar/gkx716/4080665/Transcriptioninduced-supercoiling-explains (+journal cover)

[25] **Racko D**, Benedetti F, Dorier J, Burnier Y, Sasiak A: "Molecular dynamics simulation of supercoiled, knotted and catenated DNA molecules, including modeling of action of DNA gyrase." Bacterial nucleotide, Methods in Molecular Biology vol 1624, ISBN 978-1-4939-7097-1, pp. 263-299 Humana Press, Springer (2017) http://www.springer.com/de/book/9781493970971



[24] Eric J. Rawdon, Julien Dorier, **Dusan Racko**, Kenneth C. Millett, Andrzej Stasiak: How topoisomerase IV can efficiently unknot and decatenate negatively supercoiled DNA molecules without causing their torsional relaxation. Nucleic Acids Research 04/2016; 44(10). DOI:10.1093/nar/gkw311 (+journal cover)

[23] **Dusan Racko**, Fabrizio Benedetti, Julien Dorier, Yannis Burnier, Andrzej Stasiak: Generation of supercoils in nicked and gapped DNA drives DNA unknotting and postreplicative decatenation. Nucleic Acids Research 07/2015; DOI:10.1093/nar/gkv683



[22] **Dušan Račko**, Peter Cifra: Arm retraction and escape transition in semi-flexible star polymer under cylindrical confinement. Journal of Molecular Modeling 07/2015; 21(7). DOI:10.1007/s00894-015-2735-9

[21] Fabrizio Benedetti, Aleksandre Japaridze, Julien Dorier, **Dusan Racko**, Robert Kwapich, Yannis Burnier, Giovanni Dietler, Andrzej Stasiak: Effects of physiological selfcrowding of DNA on shape and biological properties of DNA molecules with various supercoiling. Nucleic Acids Research 03/2015; 43. DOI:10.1093/nar/gkv055

[20] Klaudia Czaniková, Igor Krupa, **Dušan Račko**, Vasilij Šmatko, Eva M Campo, Ewa Pavlova, Mária Omastová: In situ electron microscopy of Braille microsystems: Photoactuation of ethylene vinyl acetate/carbon nanotube composites. Materials Research Express 02/2015; 2. DOI:10.1088/2053-1591/2/2/025601

[19] **Dušan Račko**: „The free volume of condensed phases confined in a nanopore as seen by computer simulations and compared to PALS“ Acta Physica Polonica A 125(3) 785-789 (2014).

[18] Czanikova, Klaudia; Torras, Nuria; Esteve, Jaume; **Račko Dušan** et al., Nanocomposite photoactuators based on an ethylene vinyl acetate copolymer filled with carbon nanotubes, SENSORS AND ACTUATORS B-CHEMICAL Volume: 186 Pages: 701-710 Published: SEP 2013

[17] **Račko, Dušan**; Cifra, Peter, Segregation of semiflexible macromolecules in nanochannel, JOURNAL OF CHEMICAL PHYSICS Volume: 138 Issue: 18 Article Number: 184904 Published: MAY 14 2013

[16] Danko, Martin; Andicsova, Anita; Hrdlovic, Pavol, **Račko Dušan**; et al., Spectral characteristics of carbonyl substituted 2,2 '-bithiophenes in polymer matrices and low polar solvents, PHOTOCHEMICAL & PHOTOBIOLOGICAL SCIENCES Volume: 12 Issue: 7 Pages: 1210-1219 Published: 2013

[15] **Račko, Dušan**; Kristiak, Jozef: “The Free Volume Dynamics”, Materials Science Forum Volume: 733 Pages: 33-37 Published: 2013

[14] **Račko Dušan**, On the relationship of the relative intensity I-3 and a cavity number as obtained from computer simulations, Materials Science Forum Volume: 733 Pages: 183-189 Published: 2013-

[13] Krupa I.; Nedelčev T.; Chorvát D Jr.; **Račko D.**; Lacík I.; „Glucose diffusivity and porosity in silica hydrogel based on organofunctional silanes“ Eur. Polym J. 47(7), 1477-1484 (2011).

[12] **Račko D**.; Capponi S.; Alvarez F.; et al., “The free volume of poly(vinyl methylether) as computed in a wide temperature range and at length scales up to the nanoregion” J. Chem Phys, 134(4), 044512 (2011).

[11] Krupa I.; Nedelčev T.; **Račko D.**; et al. “Mechanical properties of silica hydrogels prepared and aged at physiological conditions: testing in the compression mode” J. Sol-Gel Sci. Technol., 53(1), 107-114 (2010).

[10] **Račko D.**: “A Computational Model for Nano Scale Cavities in the Atomic Structure of Polymer Melt and Comparisons to PALS”, Mat. Sci. Forum, 666, 15-20 (2011).

[9] **Račko D.**; Capponi S.; Alvarez F.; et al.; “The free-volume structure of a polymer melt, poly(vinyl methylether) from molecular dynamics simulations and cavity analysis” J. Chem Phys., 131(6), 064903 (2009).

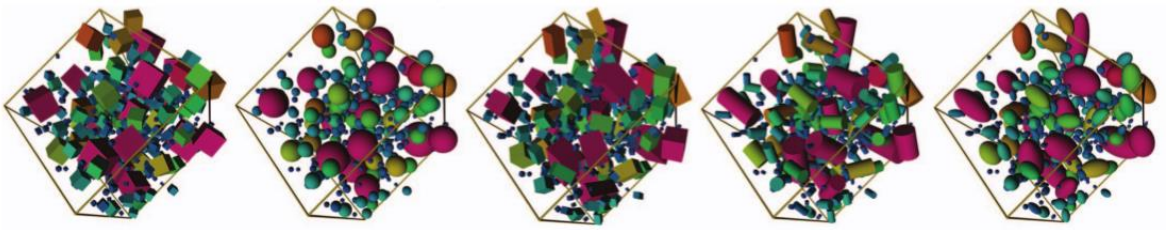
[8] Danko M.; Libiszowski J; Wolszczak; **Račko D.**; et al.; “Fluorescence study of the dynamics of a star-shaped poly(epsilon-caprolactone)s in THF: A comparison with a star-shaped poly(L-lactide)s” Polymer, 50(10), 2209-2219 (2009).

[7] Švajdlenková H.; **Račko D**.; Bartoš J.; “Spin probe reorientation and its connections with free volume and relaxation dynamics: Diglycidyl-ether of bis-phenol A” J. Non-Crys. Sol., 354(17), 1855-1861 (2008).

[6] Nedelčev T.; **Račko D.**; Krupa I.; “Preparation and characterization of a new derivative of rhodarnine B with an alkoxysilane moiety”, Dyes and pigments, 76(2), 550-556 (2008).

[5] **Račko D.**; Chelli R.; Cardini G.; et al.; “Free volume from molecular dynamics simulations and its relationships to the positron annihilation lifetime spectroscopy” Theo. Chem Acc., 118(2), 443-448 (2007).

[4] Bartoš J.; **Račko D**.; Šauša O.; et al “Positron annihilation lifetime spectroscopy and atomistic modeling - Effective tools for the disordered condensed system characterization”, SOFT MATTER UNDER EXOGENIC IMPACTS, NATO Science Series II – Mathematics, Physiscs and Chemistry, 242, 113-131 (2007).



[3] Bartoš J.; Andreozzi L; Faetti M.; Šauša O.; **Račko D.**; et al; “Free volume in poly(propylene glycol) and its relationships to spin probe reorientation” J. Non-Cryst Sol., 352(42-49) SI, 4785-4789 (2006).

[2] Bartoš J; Šauša O.; **Račko D.**; et al “Positron annihilation lifetime response and relaxation dynamics in glycerol” J. Non-cryst Sol. 351(33-36), 2599-2604 (2005).

[1] **Račko D.**; Chelli R.; Cardini G.; et al. “Insights into positron annihilation lifetime spectroscopy by molecular dynamics simulations - Free-volume calculations for liquid and glassy glycerol” Eur. Phys J D, 32(3), 289-297 (2005).

Konferencie:

[1] J. Kuriplach, **D. Račko**, J. Bartoš, O. Šauša, J. Krištiak: „Calculation of positron Llifetime of amorphous solids.“ The 1st International Workshop on Positron as a probe of condensed matter, Smolenice, Slovak Republic, 27.- 30. May 2001 (Poster)

[2] J. Bartoš, **D. Račko**, O. Šauša, J. Krištiak, D. Chorvát: „Free volume in glycerol from modeling by energy minimization.“ The 1st International Workshop on Positron as a probe of condensed matter. Smolenice, Slovak Republic, 27.- 30. May 2001 (Poster)

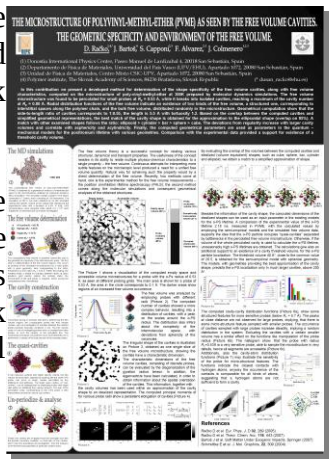
[3] **D. Račko**, „The hydrogen bonding in Glycerol“, The student’s scientific conference, April, 2002, Department of Chemistry, Commenius University, Slovak Republic (poster)

[4] **D. Račko**: „Country Report on Computational Chemistry“ and „Case study: Hydrogen Bonding in Liquid Glycerol“, Training course on Molecular Design and Computer Assisted Combinatorial Chemistry, Trieste, Italy, 9-12 July 2002 (Lectures)

[5] **D. Račko**: „The free volume: A Molecular Dynamics Insight into Positron Annihilation Lifetime Spectroscopy“, http://www.lens.unifi.it/index.php?p=seminars.ins, LENS Aula Querzoli, Florence, Italy, 17 November 2003 (Lecture)

[6] J. Bartoš, O. Šauša, J. J. Fontanella, **D. Račko**, J. Krištiak: „Positron annihilation lifetime response and relaxation dynamics by the broadband dielectric spectroscopy in glycerol.“, Book of Abstracts of the 3rd International Conference on Broadband Dielectric Spectroscopy and Its Applications. Delft, The Netherlands, 23-26 August 2004 p.160 (poster)

[7] **D. Račko**, J. Bartoš, „Free-volume microstructure of the condensed phase from computer simulations“, The 3rd Czech and Slovak Days on Polymers, POLYMÉRY 2004, Smolenice, Slovak Republic, 26-29 September 2004 (Poster)



[8] J. Bartoš, **D. Račko**, R. Chelli, G. Cardini, S. Califano: „Free volume microstructure from positron annihilation lifetime spectroscopy, free volume models and atomistic modelling and its relationships to dynamics and transport properties“, Abstract book of International meeting on polymer modelling and its industrial applications, Boras, Sweden, 7-8 June, 2005 (Poster)

[9] J. Bartoš, J. J. Fontanella, O. Šauša, J. Krištiak, L. Andreozzi, **D. Račko**: „Free volume from PALS and its relationships to the dynamic and ion transport properties in undoped and doped poly(propylene glycol)“, Abstract book of the 6th Liquid Matter Conference, Utrecht, The Netherlands, 2-6 June, 2005 (Poster)

[10] **D. Račko**, J. Bartoš, R. Chelli, G. Cardini a S. Califano: „Free volume microstructure from molecular dynamics and its relationships to the PALS and dynamic properties“, Abstract book of the 5th International Discussion Meeting on Relaxations in Complex Systems, Lille, France, 7-13 July, 2005 (Poster)

[11] J. Bartoš, L. Andreozzi, M. Faetti, O. Šauša, J. Krištiak, **D. Račko**, „The free volume in poly(propyleneglycol) and its relationships to the spin probe reorientation“, Abstract

book of the 5th International Discussion Meeting on Relaxations in Complex Systems, Lille, France, 7-13 July, 2005 (Poster)

[12] T. Nedelčev, I. Krupa, **D. Račko**, "Preparation and characterization of a new derivative of Rhodamine B with alkoxysilane moiety", Advanced Polymeric Materials APM-2006, Bratislava, Slovak Republic, 11-15 June, 2006 (Poster)

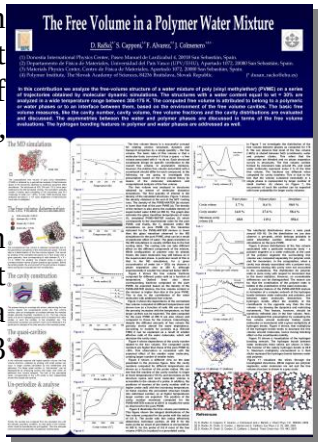
[13] J. Bartoš, L. Andreozzi, O.Šauša, M.Faetti, **D. Račko**, F.Zulli, J.Krištiak, "Crossover phenomena in glass - forming liquids as detected by PALS and ESR methods", Pisa, Italy, September 17-22, 2006 (Poster)

[14] T. Nedelčev, **D. Račko**, I. Krupa, "Preparation and characterization of a new derivative of Rhodamine B with alkoxysilane moiety", Smolenice, Slovak Republic, November 27-29, 2006 (Poster)

[15] H. Švajdlenková, I. Quintana, V. Majerník, A. Arbe, **D. Račko**, O. Šauša, J. Krištiak, J. Colmenero and J. Bartoš, "Spin probe reorientation in relation to free volume and phenyl ring dynamics in poly(ethersulphone)", XXII International EPR Seminar, Kočovce, Slovak Republic, May 30 - June 2, 2007 (Poster)
[16] J. Mosnáček, J. Kollár, J. Kronek, **D. Račko**, Cs. Kósa, M. Danko, A. Bílešová, "Aromatic Initiators For Nitroxide Mediated LFRP Synthesis And Molecular Modeling", European Polymer Congress, Portorož, Slovenia, July 2 - 6, 2007 (Poster), P1.4.83 (poster)

[17] M. Danko, J. Libiszowski, M. Wolszczak, **D. Račko**, A. Duda, "Fluorescence Study Of The Molecular Dynamics Of Star-Tetrahydrofuran As Solvent", European Polymer Congress, Portorož, Slovenia, July 2 - 6, 2007, P1.4.90 (Poster)

[18] **D. Račko**, J. Bartoš, "Free Volume Microstructure from Computer Simulations - A Straightforward Method for A Direct Free Volume Determination and Analysis", The 3rd Workshop of Young European Scientists (YES), July 8-13 2007, Krakow, Poland (Poster and Lecture)



[19] **D. Račko**, J. Bartoš, "Free Volume Microstructure from Computer Simulations - A Straightforward Method for A Direct Free Volume Determination and Analysis", The 1st Bratislava Young Polymer Scientists workshop (BYPOS), August 20-23 2007, Smolenice, Slovak Republic (Poster and Lecture)

[20] **D. Račko**, "Free Volume Microstructure from Computer Simulations (Part 1) - The Method" and "Free Volume Microstructure from Computer Simulations (Part 2) - The PBD Case", 11. September 2007, A seminar at Donostia International Physics Centre, Donostia-San Sebastian, España (lectures)

[21] **D. Račko**, J. Bartoš, S. Capponi, F. Alvarez, J. Colmenero, "The Microstructure of Poly-(vinylmethylether) as Seen by the Free Volume Cavities. The Geometrical Specificity and Environment of the Free Volume.", The 10th Granada Seminar on the Computational Physics, 15-19 September 2008, University of Granada, Granada, España" (poster)

[22] **D. Račko**, S. Capponi, F. Alvarez, J. Colmenero and J. Bartoš, The Effect of temperature on the free volume measures in polymer: PVME, The 6th IDMRCS, 31. August – 4. September 2009, Roma, Italy (poster)

[23] **D. Račko**, S. Capponi, F. Alvarez, J. Colmenero, The Free Volume in Polymer Water Mixture, CONFIT 2010, 2 – 5 March 2010, Grenoble, France (poster)

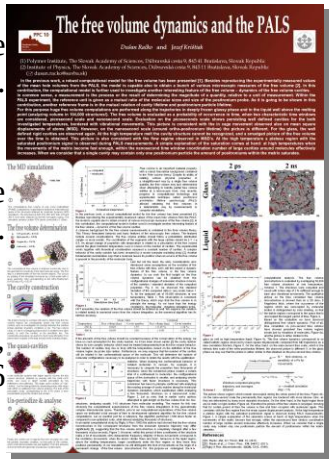
[24] **D. Račko**, The Free Volume of PVME as Computed in a Range of Temperatures and Length Scales up to the nano Region, 39th Seminar on the Positron Annihilation, PSPA10, 20-25 June 2010, Kazimiers, Poland (lecture)

[25] **D. Račko**, "Free volume in polymer water mixture", Simulating Soft Matter with ESPResSo (CECAM), 11.-15. October, 2010, Stuttgart, Germany (Poster)

[26] **D. Račko**, Computer Simulations and Discovery – Explorations behind the Free volume theory, 5.october 2010, Polymer institute of the Slovak Academy of Sciences, Bratislava (lecture)

[27] **D. Račko**, What can we learn from various free volume properties as obtained from computer simulations of polymer condensed phases, 24-27. May 2011, Mainz Materials Simulations Days 2011, Mainz, Germany (lecture&poster)

[28] **D. Račko**, The free volume in polymer water mixture, The 10th International Workshop on Positronium Chemistry, 5.-9. September 2011, Smolenice, Slovak Republic (lecture).



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[30] **D. Račko**, International Summer school on Polymers, Congress Center of the Slovak Academy of Sciences, 22-26 August 2011, Smolenice, Slovakia (lecture)

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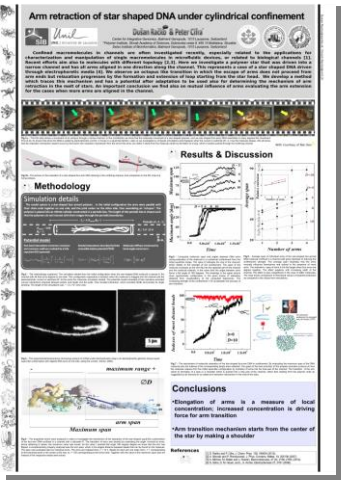

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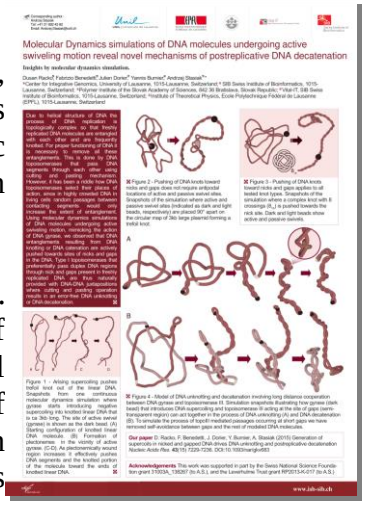
Molecular Dynamics simulations of DNA molecules undergoing active swiveling motion reveal novel mechanisms of postreplicative DNA decatenation

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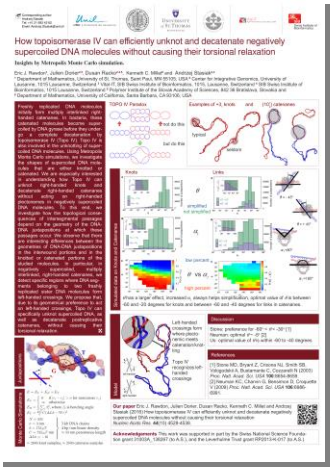
How topoisomerase IV can efficiently unknot and decatenate negatively supercoiled DNA molecules without causing their torsional relaxation

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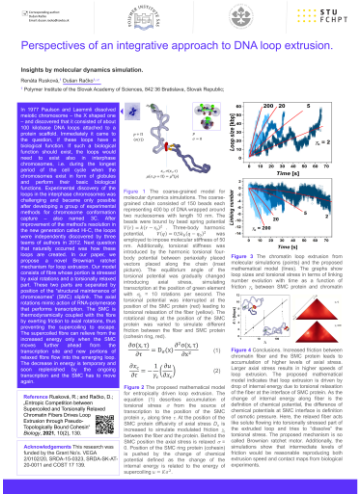
Perspectives of an integrative approach to DNA loop extrusion.

Insights by molecular dynamics simulation.

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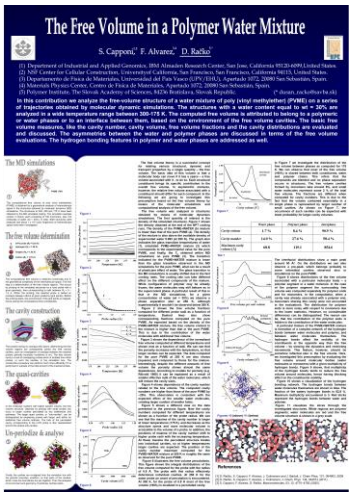

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[88] **D. Racko** "Chromatin Loop Extrusion and Chromatin Unknotting" The 1st EUTOPIA COST Action Meeting, ECT* Villa Tambosi, 4.-9. February 2019, Trento, Italy

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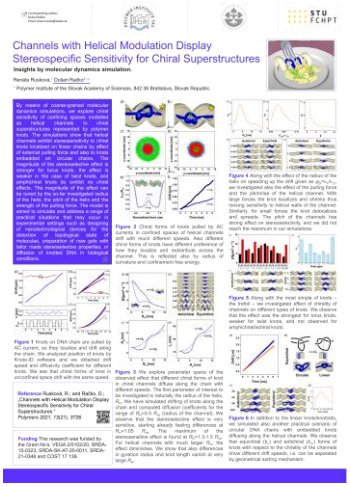
Channels with Helical Modulation Display Stereospecific Sensitivity for Chiral Superstructures

Insights by molecular dynamics simulation.

[90] **D. Racko** Introducing Supercoiling Into Models Of DNA And Chromosome Structure. XXXIII Bratislava International Conference on Macromolecules BIMac2019, Falkensteiner Hotel, Pilarikova 5, 811 03 Bratislava, 30. June-3. July 2019, Slovakia

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[98] **D. Racko** and R. Ruskova, "Coarse Grained Simulations of Bio-polymers" Open Door Sessions at Polymer Institute SAS 2020, virtual presentations https://fb.watch/1N7AFXN52C/ (lecture)

[99] **D. Racko** "Towards loop extrusion with pseudo-topologically and non-topologically bound SMC's" Eutopia 3 – Third Meeting of the European Topology Interdisciplinary Initiative
15-17 FEBRUARY 2021. FCUL, Lisbon, Portugal – as online conference. (lecture)

[100] **D. Racko** "Free Volume in Polymer Water Mixture" Interdisciplinary Challenges in Nonequilibrium Physics, April 12, 2021 - April 16, 2021, CECAM-AT/ESI, Erwin Schroedinger Institute / Technische Universität Wien (poster)

[101] R. Ruskova, **D. Racko** "Chiral knots display symmetry breaking in helical confinement" April 12, 2021 - April 16, 2021, CECAM-AT/ESI, Erwin Schroedinger Institute / Technische Universität Wien (poster)

[102] R. Ruskova, **D. Racko** "Entropic competition between supercoiled and torsionally relaxed fibers drives chromatin loop extrusion." In PREVEDA : interaktívna konferencia mladých vedcov 2021. Book of abstracts. - Banská Bystrica : Občianske združenie Preveda, 2021, abstract no. 2129. ISBN 978-80-972360-7-6. (Interaktívna konferencia mladých vedcov 2021 : PREVEDA. Interaktívna konferencia mladých vedcov 2021 : PREVEDA) (poster)

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[108] Renáta Rusková, **Dušan Račko** "Young modeller´s forum, Molecular Graphics and Modelling Society, University of Oxford, Oxford OX2 6QA, United Kingdom, 2 February 2022 Book of Abstracts: https://www.mgms.org/WordPress/wp-content/uploads/2022/01/YMF2021-22_programme.pdf#page=4 (P)

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[110] Renáta Rusková, **Dušan Račko** "Channels with helical modulation display stereosensitivity for chiral superstructures" European Polymer Congress in Prague, Prague Congresss Center, 5. května 1640/65, Nusle, 140 00 Prague 4, 26 June - 1 July 2022) p. 891 Book of Abstracts: ISBN 978-80-88214-33-5 (V)

[111] Renáta Rusková and **Dušan Račko** "HPC in design of devices for chiral nanotechnology" Austrian-Slovenian HPC Meeting 2022 – ASHPC22, organized by EuroCC Austria, c/o Universität Wien, Archkogl 31, 8993, Grundlsee, Austria, May 31 – June 2, 2022 Book of Abstracts: DOI: https://doi.org/10.25365/phaidra.337 Book of Abstracts: ISBN: 978-3-200-08499-5 (online) (P)

[112] **Dušan Račko** "The free volume in PVME-water mixture as obtained from HPC simulations" Austrian-Slovenian HPC Meeting 2022 – ASHPC22, organized by EuroCC Austria, c/o Universität Wien, Archkogl 31, 8993 Grundlsee, Austria, May 31 – June 2, 2022 Book of Abstracts: DOI: https://doi.org/10.25365/phaidra.337 ISBN: 978-3-200-08499-5 (P)

[113] RUSKOVÁ, Renáta - **RAČKO, Dušan**. Channels with helical modulation display stereosensitivity for chiral superstructures. In Polymers : 12 Czech - Slovak Conference : book of abstracts. - Prague, Czech Republic : IMC, 2022, p. [49]. ISBN 978-80-85009-96-5. (Polymers : 12 Czech - Slovak Conference. Polymers : 12 Czech - Slovak Conference) Typ: AFG (P)

[114] **RAČKO, Dušan** "DNA shape analyses and protein-DNA interaction" Integrative approach to the theoretical study of chromatin, University of Zaragoza, CECAM-ES, Río Ebro Campus, C/ Mariano Esquillor S/N, 5018 Zaragoza, Spain, May 31, 2022 - June 2, 2022 Program online: https://www.cecam.org/workshop-details/43 (P)

[115] RUSKOVÁ, Renáta - **RAČKO, Dušan**. Channels with helical modulation display stereosensitivity for chiral superstructures. The 1st Vienna Soft Matter Day 2022, Raiffeisen Lecture Hall, Koesterneuburg, Austria, 21 October 2022 Details online: https://viennasoftmatterday.pages.ist.ac.at/ (V)

[116] RUSKOVÁ, Renáta - **RAČKO, Dušan**. Knot Factories with Helical Geometry Enhance Knotting and Impose Handedness to the Knots. The 1st Vienna Soft Matter Day 2022, Raiffeisen Lecture Hall, Kloesterneuburg, Austria, 21 October 2022 Details online: https://viennasoftmatterday.pages.ist.ac.at/ (V)

[117] **RAČKO, Dušan** "Simulating topoisomerases, gyrases, polymerases and chiral confinements in Extensible Simulation Package for Research on Soft Matter (ESPResSo)" Simulating the dynamics of soft matter with ESPResSo, PyStencils and LbmPy, CECAM-DE-SMSM, Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany, 10 – 14 October 2022 Details online: https://www.cecam.org/workshop-details/1146 (V)

[118] **Racko D.** "Nano-channels with Helical Geometry Display Stereospecific Sensitivity and Induce Handedness to Chiral Superstructures" "Emerging colloidal dynamics away from equilibrium. Chiral active systems." CECAM 1-3 March 2023, Lausanne, Switzerland (poster)

[119] **Racko, D.** "Molecular Simulations of DNA Topology" STSM /EUTOPIA 17139, Department of Physics, University of Trento, Italy 19 – 26 March 2023 (lecture / seminar)

[120] Ruskova, R.; **Racko D.** "Knot Factories with Helical Geometry Enhance Knotting and Induce Handedness to Knots", Topological Soft Matter, Higgs Center, Edinburgh, Scotland, United Kingdom 10-12 May 2023 (poster)

[121] **Racko D** "Polymers with active chiral topology and nanotechnology" Topological Soft Matter, Higgs Center, Edinburgh, Scotland, United Kingdom 10-12 May 2023 (poster)

[122] **Racko, D** "Molecular simulations of DNA polymer with active topology" Polymer Meeting 15, 4 – 7 September Bratislava, Slovak Republic (invited lecture)

[123+] Racko D, Bypos 2023, Polymery 2023, ESPResSo Workshop 2023..

Koordinácia projektov (vedúci projektu):

[6] STSM COST 17135 "HELITOP" 19 March – 26 March 2023, Department of Physics, University of Trento

[5] SK-AT-20-0011"Towards Experimental Realization of Active Topological Glass" 01/04/2021-31/12/2022

[4] VEGA 2/0102/20 "Molecular dynamics simulations of topologically constrained and confined polymers" 1.1.2020/30.12.2023

[3] STSM 44913 / CA 17139 “Transcription induced supercoiling in 4D genome organization” 11.8.2019/25.8.2019

[2] VEGA 2/0068/13 “Nanostructured polymers and polymer nanostructures”, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, 841 14 Bratislava, Slovakia (01/01/2013-31/12/2016)

[1] Marie Curie Training Fellowship “Free volume from computer simulations” within HPMT-CT-2000-00123 European laboratory for Non-Linear Spectroscopy, Largo E. Fermi 2, Università di Firenze, 50125 FIRENZE, Italy (01/05/2003-01/05/2004)

Zaslané projekty

[1] VEGA 2/0038/24 “PACT NANOTEC”

Zamietnuté projekty

[4] APVV-20-0525 a project on crosslinking in pores 2021

[3] JRDF 201307832 a project on diffusion and kinetics 2019

[2] A project on computer simulations of DNA and chromatin in different topological conditions and development of new computational models submitted to Marie Curie Sklodowska Actions within the H2020, Individual Fellowships / Reintegration Panel (2019).

[1] A project on free volume simulations of condensed phases and development of computational tools for the free volume analysis submitted to Marie Curie Sklodowska Actions within the 6th Framework Program, Individual fellowships / Standard panel (2006).

Spolupráca na projektoch:

[15] APVV-21-0355, Changes of microstructure and physical properties of crosslinked polymers in bulk and under confined conditions of macro- and mesopores 2022 - 2027

[14] APVV-21-0346, Modification of surfaces as barrier to protein adsorption 2022 – 2027.

[13] COST 17139 European Topology Interdisciplinary Action (EUTOPIA) Luca Tubiana (Uni Trento) 2018-2023

[12] APVV-16-0369 “Physical properties of organic compounds and water confined in mesopores of inorganic matrices” (01/07/2017-30/06/2021, principal investigator Ondrej Sausa)

[11] APVV-15-0323 “Structural transitions of (bio)macromolecules in nanochannels” (01/07/2016-30/06/2020, principal investigator Peter Cifra)

[10] APVV-11-0451 „Nanostructure in macromolecular systems induced by confinement“, (26/03/2015-25/03/2018, principal investigator Peter Cifra)

[9] MACHINA (Stage II.), Center for materials, layers and systems for applications and chemical processes under extreme conditions Stage II, which is supported by the Research & Development Operational Program and funded by the ERDF 2010-2013.

[8] EC228916/ FP7-NMP-2008-SMALL-2, collaboration on “Nano-Optical Mechanical Systems (NOMS)” within the 7th Framework Program “FP7-NMP - Specific Programme "Cooperation": Nanosciences, Nanotechnologies, Materials and new Production Technologies” (2009-2012)

[7] VEGA 2/0093/12 „Structural transitions of confined semi-flexible macromolecules“ (principal investigator Peter Cifra)

[6] MACHINA (Stage I.), Centre for materials, layers and systems for applications and chemical
processes under extreme conditions supported by the Research & Development Operational Program funded by the ERDF, 2007-2010.

[5] No. IT-436-07 Basque Government and Spanish MEC Grant No. CSD2006-53 (principal investigator Juan Colmenero de Leon)

[4] MAT2007-63681 Spanish Ministry of Education, Donostia International Physics Center (principal investigator Juan Colmenero de Leon)

[3] APVT 51-045302, “Free volume of molecular and polymer systems and their transport and dynamic properties.” (principal investigator J. Kristiak)

[2] APVT-51-004904 „New aromatic nitroxides and alkoxyamines. Synthesis, characterization and use in LFPR and stabilization of polyolefins“ 2004-2007 (principal investigator Jaroslav Mosnáček)

[1] HPMT-CT-2000-00123 “Cold atoms and quantum degeneracy”, Human Resources and Mobility, FP5-Human potential: Programme for research, technological development and demonstration on "Improving the human research potential and the socio-economic knowledge base", European laboratory for Non-Linear Spectroscopy, Largo E. Fermi 2, Università di Firenze, 50125 Florence, Italy (01/09/2000-31/08/2004)

Kurzy:

[41] VSC/EuroCC ONLINE BOOTCAMP - EuroCC N-Ways to GPU Programming Bootcamp, May 15-16, 2023

[40] VSC/EuroCC HYBRID COURSES: Parallel programming with MPI and/or OpenMP, April 24-28, 2023

[39] VSC/EuroCC WEBINAR - Superpower for the Power Grid, March 29-30, 2023

[38] VSC ONLINE COURSE - Python for HPC, February 22-23, 2023

[37] VSC ONLINE COURSE - Python for HPC, Vienna Supercomputer Cluster, University of Vienna, December 6-7, 2022

[36] VSC HYBRID COURSE - Parallelization with MPI, Vienna Supercomputer Cluster, University of Vienna, November 22-25, 2022

[35] VSC ONLINE COURSE - CUDA 4 Dummies, Vienna Supercomputer Cluster, University of Vienna, October 24-25, 2022

[34] CECAM, Simulating the dynamics of soft matter with ESPResSo, PyStencils and LbmPy, CECAM-DE-SMSM, Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany, 10 – 14 October 2022

[33] VSC ONLINE COURSES - VSC-Linux (October 18, 2022) + VSC-Intro, Vienna Supercomputer Cluster, University of Vienna, October 21, 2022

[32] ITKurzy SAV, Online Technology transfer workshop with University of Edinburgh, May 20 2022

[31] ITKurzy SAV, Úvod do aplikácií zložitých výpočtov v medicíne, Oddelenie počítačovej grafiky a videnia, Katedra aplikovanej informatiky, FMFI UK, 12 April 2022

[30] VSC ONLINE COURSE - Hybrid Programming in HPC - MPI+X, Vienna Supercomputer Cluster, University of Vienna, April 05-07, 2022

[29] ITKUrzy SAV, Modelovanie elektrónových vlastností 2D systémov metódami kvantového Monte Carla, 15 February 2022

[28] Matural and artificial intelligence, ITKurzy 24. May 2022

[27] Application of HPC computing in medicin, ITKurzy 12. April 2022

[26] Deep learning for computer seeing, ITKurzy 29. March 2022

[25] Introduction to artificial neural networks and evolutionary algorithms, ITKurzy 15. March 2022

[24] Course on HPC infrastructure, ITKurzy SAS, 13. May 2022

[23] Entanglement Days of Biopolymers (22-26 June 2021) Virtual workshop on entangled biomolecules, University of Warsaw (online)

[22] EUTOPIA Software Training Series #4 “Topological analysis” (online)
• Part 1 - Introduction to topological analysis (June 17-18) Pawel Dabrowski-Tumanski
• Part 2 - Virtual workshop on entangled biomolecules (June 24-25)
• Part 3 - KnotoID and Surface Evolver (July 1-2)

[21] ONLINE COURSE - Parallel I/O, May 18-19, 2021 University of Vienna

[20] EUTOPIA Software Training Series #3 All atom DNA simulations. 29-30th April 2021 (Agnes Noy / Sarah Harris) (online)

[19] EUTOPIA Software Training Series #2 “Analysis of MD Trajectories.” 25-26 March 2021 (Marco Giulini, Samuela Pasquali, Pawel Dabrowski-Tumanski) (online)

[18] EUTOPIA Software Training Series #1 “Molecular Dynamics and LAMMPS.” 25-26 February 2021 (Davide Michieletto) (online)

[17] CADMOS HPC Course 2018, Hôtel Suisse in Champéry, Switzerland, 9.-11. July 2018

[16] 5th Lausanne CompBio Meeting, Meeting of various UNIL/EPFL groups that are active in research related to Computational Biology, November 30 2017, Auditorium “C”, Building Genopode, Universite de Lausanne, Lausanne, Switzerland.

[15] 4th Lausanne CompBio Meeting, Meeting of various UNIL/EPFL groups that are active in research related to Computational Biology, May 30 2017, Auditorium “Charlotte Olivier”, main building of the Central University Hospital of Vaud (CHUV), Lausanne, Switzerland.

[14] 3rd Lausanne CompBio Meeting, Meeting of various UNIL/EPFL groups that are active in research related to Computational Biology, January 18 2017, Auditorium at Biophore, University of Lausanne, Lausanne, Switzerland.

[13] 2nd Lausanne CompBio Meeting, Meeting of various UNIL/EPFL groups that are active in research related to Computational Biology, September 14 2016, Auditorium at Biophore, University of Lausanne, Lausanne, Switzerland.

[12] 1st Lausanne CompBio Meeting, Meeting of various UNIL/EPFL groups that are active in research related to Computational Biology, May 3 2016, Auditorium “Maternity”, Central University Hospital of Vaud (CHUV), Lausanne, Switzerland.

[11] High Performance Computing in Life Sciences, Infrastructure training, Vital-IT Swiss Institute Bionformatics, Center of Integrative Genomics, Genopode, 11. February 2015, Lausanne, Switzerland.

[10] 2nd High-Performance Computing workshop, 11-13. November 2013, Congress Center of the Slovak Academy of Sciences

[9] 1st High-Performance Computing workshop, 21.-22. November 2012, Congress Center of the Slovak Academy of Sciences

[8] ESPResSo Summer School (CECAM). 8.-12 October 2012, Stuttgart, Germany

[7] Simulating Soft Matter with ESPResSo, University of Stuttgart, 11.-15. October, Stuttgart, Germany

[6] 2nd International Workshop on Grid Computing for Complex Problems, Institute of Informatics, Slovak Academy of Sciences, 28-30 November 2006, Bratislava, Slovakia

[5] 1st International Workshop on Grid Computing for Complex Problems, Institute of Informatics SAS, 29-30 November 2005, Bratislava, Slovakia

[4] Developing skills for future career under EC FP7, the Slovak Academic Information Agency

[3] TRVS XI “Time resolved vibrational spectroscopy”, May 24-29 2003, Castiglione della Pescaia, Italy.

[2] Training course on Molecular Design and Computer Assisted Combinatorial Chemistry, Trieste, Italy, 9-12 July 2002.

[1] Courses of English language at the Institute of Languages, Slovak Academy of Sciences (October 2000 – May 2001)

Bratislava, 01.05.2023 Dušan Račko