



Dynamics of Complex Continua

Results

Project Information

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[Project website](#) 

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Coordinated by

UNIVERSITÄT INNSBRUCK



Austria

CORDIS provides links to public deliverables and publications of HORIZON projects.

Links to deliverables and publications from FP7 projects, as well as links to some specific result types such as dataset and software, are dynamically retrieved from [OpenAIRE](#) .

Publications

[Peer reviewed articles \(28\)](#)



[Data-Proximal Complementary \$\ell_1\$ -TV Reconstruction for Limited Data Computed Tomography](#) 

Author(s): Simon Göppel, Jürgen Friel, Markus Haltmeier

Published in: Mathematics, Issue 12, 2024, Page(s) 1606, ISSN 2227-7390

Publisher: MDPI

DOI: 10.3390/math12101606

[Evolution of the Immunoglobulin Isotypes—Variations of Biophysical Properties among Animal Classes](#) 

Author(s): Nancy D. Pomarici; Roberta Cacciato; Janik Kokot; Monica L. Fernández-Quintero; Klaus R. Liedl

Published in: Biomolecules, Issue 13 (5), 2023, Page(s) 801, ISSN 2218-273X

Publisher: MDPI AG 2011

DOI: 10.3390/biom13050801

[Semi-Lagrangian 4d, 5d, and 6d kinetic plasma simulation on large-scale GPU-equipped supercomputers](#) 

Author(s): Lukas Einkemmer; Alexander Moriggl

Published in: The International Journal of High Performance Computing Applications, Issue 37 (2), 2022, Page(s) 180-196, ISSN 1741-2846

Publisher: Sage Publishing

DOI: 10.1177/10943420221137599

[On the Subparsec-scale Core Composition of FR 0 Radio Galaxies](#) 

Author(s): Margot Boughelilba; Anita Reimer

Published in: The Astrophysical Journal Letters, Issue 955 (2), 2023, Page(s) L41, ISSN 2041-8213

Publisher: IOP Publishing

DOI: 10.3847/2041-8213/acf83c

[Feature Reconstruction from Incomplete Tomographic Data without Detour](#) 

Author(s): Simon Göppel; Jürgen Friel; Markus Haltmeier

Published in: Mathematics, Issue 10 (8), 2022, Page(s) 1318, ISSN 2227-7390

Publisher: MDPI

DOI: 10.3390/math10081318

[Modelling the impact of argon atoms on a tungsten surface](#) 

Author(s): Shokirbek Shermukhamedov; Michael Probst

Published in: The European Physical Journal D, Issue 76 (169), 2022, Page(s) 9, ISSN 1434-6079

Publisher: EDP Sciences, Società Italiana di Fisica and Springer

DOI: 10.1140/epjd/s10053-022-00495-3

[An accurate and time-parallel rational exponential integrator for hyperbolic and oscillatory PDEs](#) 

Author(s): Marco Caliarì, Lukas Einkemmer, Alexander Moriggl, Alexander Ostermann

Published in: Journal of Computational Physics, Issue 437, 2021, Page(s) 110289, ISSN 0021-9991

Publisher: Academic Press

DOI: 10.1016/j.jcp.2021.110289

[A Semi-Lagrangian Discontinuous Galerkin Method for Drift-Kinetic Simulations on GPUs](#)

Author(s): Lukas Einkemmer; Alexander Moriggl

Published in: SIAM journal on Scientific Computing, Issue 46 (2), 2024, Page(s) 33-55, ISSN 0885-7474

Publisher: Kluwer Academic/Plenum Publishers

DOI: 10.1137/23m1559658

[Nonlinear mechanical model of a fluid inerter](#)

Author(s): Miriam Chillemi; Thomas Furtmüller; Christoph Adam; Antonina Pirrotta

Published in: Mechanical Systems and Signal Processing, Issue 188, 2023, Page(s) 109986, ISSN 0888-3270

Publisher: Academic Press

DOI: 10.1016/j.ymssp.2022.109986

[Sputtering from rough tungsten surfaces: Data-driven molecular dynamics simulations](#)

Author(s): Shokirbek Shermukhamedov; Michael Probst

Published in: Physics of Plasmas, Issue 30 (12), 2023, Page(s) 123901, ISSN 1070-664X

Publisher: American Institute of Physics

DOI: 10.1063/5.0167840

[Lagrangian solver for coupling hydrodynamics with biokinetic conversion modelling in anaerobic digesters](#)

Author(s): Yan, Jeremy Z.; Prashant Kumar; Nikolaus Rauch; Soroush Dabiri; Wolfgang Rauch

Published in: Water Research, Issue 252, 2021, Page(s) 121211, ISSN 0043-1354

Publisher: Elsevier BV

DOI: 10.1016/j.watres.2024.121211

[Bispecific antibodies—effects of point mutations on CH3-CH3 interface stability](#)

Author(s): Nancy D Pomarici; Monica L Fernández-Quintero; Patrick K Quoika; Franz Waibl; Alexander Bujotzek; Guy Georges; Klaus R Liedl

Published in: Protein Engineering, Design and Selection, Issue 35, 2022, ISSN 1741-0126

Publisher: Oxford University Press

DOI: 10.1093/protein/gzac012

[Corrigendum: Comparing Antibody Interfaces to Inform Rational Design of New Antibody Formats](#)

Author(s): Monica L. Fernández-Quintero; Patrick K. Quoika; Florian S. Wedl; Clarissa A. Seidler; Katharina B. Kroell; Johannes R. Loeffler; Nancy D. Pomarici; Valentin J. Hoerschinger; Alexander Bujotzek; Guy Georges; Hubert Kettenberger; Klaus R. Liedl

Published in: Frontiers in Molecular Biosciences, Issue 9, 2022, ISSN 2296-889X

Publisher: Frontiers Media S.A.

DOI: 10.3389/fmolb.2022.864654

[Electronic transitions in Rb₂⁺ dimers solvated in helium](#)

Author(s): Simon Albertini, Paul Martini, Arne Schiller, Harald Schöbel, Elham Ghavidel, Milan Ončák, Olof Echt, Paul Scheier

Published in: Theoretical Chemistry Accounts, Issue 140/3, 2021, ISSN 1432-881X

Publisher: Springer Verlag

DOI: 10.1007/s00214-021-02728-x

[Lepto-hadronic Jet-disk Model for the Multiwavelength SED of M87](#)

Author(s): Margot Boughelilba; Anita Reimer; Lukas Merten

Published in: The Astrophysical Journal, Issue 1, 2022, Page(s) 79, ISSN 1538-4357

Publisher: IOP Publishing

DOI: 10.3847/1538-4357/ac8e64

[Learning how to find targets in the micro-world: the case of intermittent active Brownian particles](#)

Author(s): Michele Caraglio; Harpreet Kaur; Lukas J. Fiderer; Andrea López-Incera; Hans J. Briegel; Thomas Franosch; Gorka Muñoz-Gil

Published in: Soft Matter, Issue 20 (9), 2024, Page(s) 2008-2016, ISSN 1744-6848

Publisher: Royal Society of Chemistry (RSC)

DOI: 10.1039/d3sm01680c

[Block preconditioning strategies for generalized continuum models with micropolar and nonlocal damage formulations](#)

Author(s): Nasser Alkmim; Peter Gamnitzer; Matthias Neuner; Günter Hofstetter

Published in: Numerical and Analytical Methods in Geomechanics, Issue 48 (7), 2024, Page(s) 1879-1906, ISSN 0363-9061

Publisher: John Wiley & Sons Inc.

DOI: 10.1002/nag.3707

[Fluid inerter-based vibration control of multi-modal structures subjected to vertical vibration](#)

Author(s): Miriam Chillemi, Thomas Furtmüller, Christoph Adam, Antonina Pirrotta

Published in: Engineering Structures, Issue Volume 307, 2024, Page(s) 117938, ISSN 0141-0296

Publisher: Pergamon Press Ltd.

DOI: 10.1016/j.engstruct.2024.117938

[Scrutinizing FR 0 radio galaxies as ultra-high-energy cosmic ray source candidates](#)

Author(s): Lukas Merten, Margot Boughelilba, Anita Reimer, Paolo Da Vela, Serguei Vorobiov, Fabrizio Tavecchio, Giacomo Bonnoli, Jon Paul Lundquist, Chiara Righi

Published in: Astroparticle Physics, Issue 128, 2021, Page(s) 102564, ISSN 0927-6505

Publisher: Elsevier BV

DOI: 10.1016/j.astropartphys.2021.102564

[Structure and Dynamics Guiding Design of Antibody Therapeutics and Vaccines](#)

Author(s): Monica L. Fernández-Quintero; Nancy D. Pomarici; Anna-Lena M. Fischer; Valentin J. Hoerschinger; Katharina B. Kroell; Jakob R. Riccabona; Anna S. Kamenik; Johannes R. Loeffler; James A. Ferguson; Hailee R. Perrett; Klaus R. Liedl; Julianna Han; Andrew B. Ward

Published in: Antibodies, Issue 12 (4), 2023, Page(s) p 67, ISSN 2073-4468

Publisher: MDPI

DOI: 10.3390/antib12040067

[Adaptive active Brownian particles searching for targets of unknown positions](#)

Author(s): Harpreet Kaur; Thomas Franosch; Michele Caraglio

Published in: Machine Learning: Science and Technology, Issue 4 (3), 2023, Page(s) 035008, ISSN 2632-2153

Publisher: IOP Publishing Ltd

DOI: 10.1088/2632-2153/ace6f4

[Experimental and numerical investigation of a fluid inerter for structural control](#)

Author(s): Miriam Chillemi; Thomas Furtmüller; Christoph Adam; Antonina Pirrotta

Published in: Journal of Sound and Vibration, Issue 573, 2024, Page(s) 118222, ISSN 0022-460X

Publisher: Academic Press

DOI: 10.1016/j.jsv.2023.118222

[Effect of turbulent diffusion in modeling anaerobic digestion](#)

Author(s): Jeremy Z. Yan; Prashant Kumar; Wolfgang Rauch

Published in: Bioresource Technology, Issue 393, 2024, ISSN 0960-8524

Publisher: Elsevier BV

DOI: 10.1016/j.biortech.2023.130068

[Modelling the sputtering and reflection from a beryllium surface: atomistic analysis](#) 

Author(s): Shokirbek Shermukhamedov, Lei Chen, Renat Nazmutdinov, Alexander Kaiser, Michael Probst

Published in: Nuclear Fusion, Issue 61/8, 2021, Page(s) 086013, ISSN 0029-5515

Publisher: Institute of Physics Publishing

DOI: 10.1088/1741-4326/ac044e

[Confinement Effect on Heterogeneous Electron Transfer in Aqueous Solutions inside Conducting Nanotubes](#) 

Author(s): Shokirbek A. Shermukhamedov, Renat R. Nazmutdinov, Michael D. Bronshtein, Michael Probst

Published in: ChemElectroChem, Issue 8/3, 2021, Page(s) 563-569, ISSN 2196-0216

Publisher: Wiley-VCH

DOI: 10.1002/celc.202001569

[Sputtering and reflection from a beryllium surface: effects of hydrogen isotope mass, impact position and surface binding energy](#) 

Author(s): S. Shermukhamedov; L. Chen; Renat Nazmutdinov; Michael Probst

Published in: Nuclear Fusion, Issue 62 (6), 2022, Page(s) 066024, ISSN 0029-5515

Publisher: Institute of Physics Publishing

DOI: 10.1088/1741-4326/ac592a

[Sputtering of the beryllium tungsten alloy Be 2 W by deuterium atoms: molecular dynamics simulations using machine learned forces](#) 

Author(s): L. Chen, A. Kaiser, M. Probst, S. Shermukhamedov

Published in: Nuclear Fusion, Issue 61/1, 2021, Page(s) 016031, ISSN 0029-5515

Publisher: Institute of Physics Publishing

DOI: 10.1088/1741-4326/abc9f4

[Translation invariant diagonal frame decomposition of inverse problems and their regularization](#) 

Author(s): Simon Göppel; Jürgen Friel; Markus Haltmeier

Published in: Inverse Problems, Issue 39 (6), 2023, Page(s) 065011, ISSN 1361-6420

Publisher: IOP Publishing

DOI: 10.1088/1361-6420/accd15

[Introducing CHAD -- An ADM1 Solver for Direct Linking to Lagrangian CFD Software](#)

Author(s): Kumar, Prashant; Yan, Zhenghao; Dabiri, Soroush; Rauch, Nikolaus; Rauch, Wolfgang

Published in: 2nd International Joint Conference on Water Distribution Systems Analysis & Computing and Control in the Water Industry, 2023, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.48550/arxiv.2311.08927

[Low-luminosity jetted AGN as particle multi-messenger sources](#)

Author(s): A. Reimer*, M. Boughelilba, L. Merten and P. Da Vela

Published in: XVIII International Conference on Topics in Astroparticle and Underground Physics (TAUP2023) - High-Energy Astrophysics and Cosmic Rays, Issue 441, TAUP2023, 2024, Page(s) 119, ISSN 1824-8039

Publisher: PoS, Sissa Medialab

DOI: 10.22323/1.441.0119

[Spine-sheath jet model for low-luminosity AGNs](#)

Author(s): Boughelilba, Margot; Reimer, Anita; Merten, Lukas; Lundquist, Jon-Paul

Published in: Proceeding of 38th International Cosmic Ray Conference (ICRC2023), Issue 958, 2023, ISSN 1824-8039

Publisher: Sissa Medialab

DOI: 10.22323/1.444.0958

[FR-0 jetted active galaxies: extending the zoo of candidate sites for UHECR acceleration](#)

Author(s): Merten, Lukas; Boughelilba, Margot; Reimer, Anita; Da Vela, Paolo; Vorobiov, Serguei; Tavecchio, Fabrizio; Bonnoli, Giacomo; Lundquist, Jon Paul; Righi, Chiara

Published in: Proceedings of 37th International Cosmic Ray Conference (ICRC2021), Issue 395, 2021, Page(s) 986, ISSN 1824-8039

Publisher: Sissa Medialab

DOI: 10.22323/1.395.0986

[Extrapolating FR-0 radio galaxy source properties from the propagation of multi-messenger ultra-high-energy cosmic rays](#)

Author(s): Jon Paul Lundquist; Lukas Merten; Serguei Vorobiov; Margot Boughelilba; A. Reimer; Paolo Da-Vela; Fabrizio Tavecchio; Giacomo Bonnoli; Chiara Righi

Published in: Proceedings of 37th International Cosmic Ray Conference (ICRC2021), Issue 395, 2022, Page(s) 989, ISSN 1824-8039

Publisher: Sissa Medialab

DOI: 10.22323/1.395.0989

[Combining Reconstruction and Edge Detection in Computed Tomography](#)

Author(s): Frikel, Jürgen; Göppel, Simon; Haltmeier, Markus

Published in: Bildverarbeitung für die Medizin 2021: Proceedings, German Workshop on Medical Image Computing, 2021, Page(s) 153-157, ISBN 978-3-658-33197-9

Publisher: Springer Fachmedien

DOI: 10.1007/978-3-658-33198-6_37

[Translation invariant diagonal frame decomposition for the Radon transform](#)

Author(s): Göppel, Simon; Haltmeier, Markus; Frikel, Jürgen

Published in: 2023 International Conference on Sampling Theory and Applications (SampTA), 2023, Page(s) 1-5, ISBN 979-8-3503-2885-1

Publisher: IEEE

DOI: 10.1109/sampta59647.2023.10301412

[CR-ENTREES -- Cosmic-Ray ENergy TRansport in timE-Evolving astrophysical Settings](#)

Author(s): Reimer, Anita; Merten, Lukas; Boughelilba, Margot; Da Vela, Paolo; Vorobiov, Serguei; Lundquist, Jon Paul

Published in: Proceedings of 38th International Cosmic Ray Conference, PoS (ICRC2023), Issue 444, 2023, Page(s) 1466, ISSN 1824-8039

Publisher: Sissa Medialab

DOI: 10.22323/1.444.1481

[Neural Network Based Molecular Dynamics Simulations of Sputtering Processes](#)

Author(s): Shokirbek Shermukhamedov; Michael Probst; Lei Chen

Published in: IEEE 17th International Conference on eScience, 2021, Page(s) 241-242, ISBN 978-1-6654-4708-9

Publisher: IEEE conference eXpress Publishing

DOI: 10.1109/escience51609.2021.00041

[Efficient Modeling of Heavy Cosmic Rays Propagation in Evolving Astrophysical Environments](#)

Author(s): Merten, Lukas; Da Vela, Paolo; Reimer, Anita; Boughelilba, Margot; Lundquist, Jon Paul; Vorobiov, Serguei; Tjus, Julia Becker

Published in: Proceedings of 38th International Cosmic Ray Conference (ICRC2023), Issue 444, 2023, Page(s) 1466, ISSN 1824-8039

Publisher: Sissa Medialab

DOI: 10.22323/1.444.1466

[The UHECR-FR0 Radio Galaxy Connection: A Multi-Messenger Study of Energy Spectra/Composition Emission and Extragalactic Magnetic Field Propagation](#)

Author(s): Lundquist, J. P.; Merten, L.; Vorobiov, S.; Boughelilba, M.; Reimer, A.; Da Vela, P.; Tavecchio, F.; Bonnoli, G.; Righi, C.

Published in: 38th International Cosmic Ray Conference (ICRC2023) - Multi Messenger and Gravitational Wave (MM&GW), Issue 444, 2023, Page(s) 1512, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.22323/1.444.1512

Other (6)

[LeXInt: GPU-accelerated Exponential Integrators package](#) 

Author(s): Deka, Pranab J.; Moriggl, Alexander; Einkemmer, Lukas

Published in: arXiv preprint, 2023, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.48550/arxiv.2310.08344

[Data-proximal null-space networks for inverse problems](#) 

Author(s): Göppel, Simon; Friel, Jürgen; Haltmeier, Markus

Published in: arXiv preprint, 2023, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.48550/arxiv.2309.06573

[Characterizing the \$\gamma\$ -ray Emission from FR0 Radio Galaxies](#) 

Author(s): Nikita S. Khatiya, Margot Boughelilba, Christopher M. Karwin, Alex McDaniel, Xiurui Zhao, Marco Ajello, Anita Reimer, and Dieter H. Hartmann

Published in: arXiv preprint, 2023, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.48550/arxiv.2310.19888

[Learning high-dimensional reaction coordinates of fast-folding proteins using State Predictive information bottleneck and Bias Exchange Metadynamics](#) 

Author(s): Nancy D. Pomarici, Shams Mehdi, Patrick K. Quoika, Suemin Lee, Johannes R. Loeffler, Klaus R. Liedl, Pratyush Tiwary, Monica L. Fernández-Quintero

Published in: bioRxiv, 2024, Page(s) 2023.07.24.550401, ISSN 2692-8205

Publisher: Cold Spring Harbor Laboratory

DOI: 10.1101/2023.07.24.550401

[Uncertainty-Aware Null Space Networks for Data-Consistent Image Reconstruction](#) 

Author(s): Angermann, Christoph; Göppel, Simon; Haltmeier, Markus

Published in: arXiv preprint, 2023, ISSN 2331-8422

Publisher: Cornell University
DOI: 10.48550/arxiv.2304.06955

[Structure to Property: Chemical Element Embeddings and a Deep Learning Approach for Accurate Prediction of Chemical Properties](#) 

Author(s): Shermukhamedov, Shokirbek; Mamurjonova, Dilorom; Probst, Michael

Published in: arXiv preprint, 2023, ISSN 2331-8422

Publisher: Cornell University

DOI: 10.48550/arxiv.2309.09355

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[Structure to Property: Chemical Element Embeddings and a Deep Learning Approach for Accurate Prediction of Chemical Properties](#) 

Author(s): Shermukhamedov, Shokirbek; Mamurjonova, Dilorom; Probst, Michael

Published in: arXiv

[Introducing CHAD -- An ADM1 Solver for Direct Linking to Lagrangian CFD Software](#) 

Author(s): Kumar, Prashant; Yan, Zhenghao; Dabiri, Soroush; Rauch, Nikolaus; Rauch, Wolfgang

Published in: arXiv

[Data-proximal null-space networks for inverse problems](#) 

Author(s): Göppel, Simon; Friel, Jürgen; Haltmeier, Markus

Published in: arXiv

[Characterizing the \$\gamma\$ -ray Emission from FR0 Radio Galaxies](#) 

Author(s): Khatiya, Nikita S.; Boughelilba, Margot; Karwin, Christopher M.; McDaniel, Alex; Zhao, Xiurui; Ajello, Marco; Reimer, Anita; Hartmann, Dieter H.

Published in: arXiv

[LeXInt: GPU-accelerated Exponential Integrators package](#) 

Author(s): Deka, Pranab J.; Moriggl, Alexander; Einkemmer, Lukas

Published in: arXiv

[Uncertainty-Aware Null Space Networks for Data-Consistent Image Reconstruction](#) 

Author(s): Angermann, Christoph; Göppel, Simon; Haltmeier, Markus
Published in: arXiv

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