# **Curriculum Vitae** of Vitaliy A Kurlin (April 2025)


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| **Title** | Professor | Computer Science department and |
| **Web** | http://kurlin.org | Materials Innovation Factory, Liverpool, UK |
| **Research** | Mathematical Data Science | crystallography, chemistry, and bioinformatics |


Since 2017 I have led a group developing a new area of Geometric Data Science to enable a transparent design of materials and molecules. The key results are the Crystal Isometry Principle and *Principle of Molecular Rigidity* based on the polynomial-time extension of the side-side-side theorem justifying the rigorous concepts of periodic and molecular structures. The current grants are the Royal Society APEX fellowship and Internation Exchanges with Prof Yoshua Bengio, a 'father' of modern AI and the Alan Turing award winner 2018.

## Higher education

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| Nov 2000 – Oct 2003 | *PhD thesis* in Geometry and Topology, Moscow State University |
| Sep 1995 – Mar 2002 | *MSc thesis* in Mathematics, Independent University of Moscow |
| Sep 1995 – Jun 2000 | *MSc thesis* in Mathematics, Moscow State University |

## Academic training

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| March – October 2021 | *Heilbron leadership programme*, University of Liverpool, UK |
| Sep 2008 – Sep 2009 | *Postgraduate Certificate* in Teaching and Learning in HE, UK |

## Employment record

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| Since September 2016 | Senior Lecturer, Reader, Professor, University of Liverpool, UK |
| Sep 2014 – Aug 2016 | Visiting scientist in Computer Vision, Microsoft, Cambridge, UK |
| Sep 2007 – Aug 2016 | Lecturer in Mathematics, Durham University, UK |
| June – Sep 2007 | Research Assistant in Sensor Networks, Lancaster University, UK |
| Sep 2005 – May 2007 | Marie Curie International Incoming Fellow, University of Liverpool |
| Feb – July 2005 | Teaching Fellow, Independent University of Moscow, Russia |
| Dec 2003 – Nov 2004 | Postdoctoral Fellow, University of Burgundy, Dijon, France |

## Teaching experience

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| Since 2019 | Developed and led the PhD training in AI and Data Science with 20 two-hour sessions per year for PhD students from the EPSRC CDT in Digital and Automated Materials Chemistry and STFC CDT on Data Intensive Science. |
| Since 2018 | Developed and taught the 15-credit module COMP229 (Introduction to Data Science), which annually attracted on average 100+ mathematics students. |
| 2017 – 2019 | Taught the industry-oriented COMP315 (technologies of e-commerce) and COMP213 (object-oriented programming) for large classes of 150+ students. |
| 2013 | *Lecturer of the Year Award* by the Student Union at Durham University. |
| 2007 – 2016 | Taught mathematics modules to large classes of up to 250 students. |

**Data Science PhD training** and COMP229 connect the latest research with innovative teaching of practical skills to extract mathematically justified insights from real data.

**International leadership**

Since 2024 Area Chair at the top Compute Science conferences NeurIPS and ICML.

Since 2023 One of 9 members in the International Union of Crystallography (IUCr) Commission on Mathematical and Theoretical Crystallography (MaThCryst).

Since 2021 Organiser of mini-symposia at the IUCr Congress 2023, SIAM Mathematical Aspects of Materials Science 2021 and 2024. Delivered the 2-hour tutorial in Geometric Data Science at the SIAM Mathematics of Data Science 2024.

Since 2020 Founder and organiser of the annual conference MACSMIN = Mathematics and Computer Science for Materials Innovation. A guest editor of the journal Acta Cryst A, which published about 10 papers presented at MACSMIN 2022.

Since 2017 Leading the LMS network Applied Geometry and Topology. Member of the American and European Math. Societies, SIAM, European Crystallographic Association, UK Higher Education Academy, EPSRC peer review college.

**Professional experience** at the University of Liverpool

Since 2017 leading the Data Science Theory and Applications group in the MIF:
8 PhD graduates since 2021, mostly employed as postdocs or permanent staff members.

**Research awards** (over £1.3M of PI's grant income for Liverpool since 2017)

2024 – 2032 Co-I in the CDT Digital and Automated Materials Chemistry, Liverpool.

2024 – 2029 Co-I in the EPSRC AI for Chemistry hub, Liverpool and Imperial College.

2024 – 2026 **Royal Society** International Exchanges with Yoshua Bengio (Montreal).
*Title:* Generative methods for materials on geographic-style maps of crystals.

2023 – 2025 **Royal Society APEX** fellowship (£100K), teaching replacement for 2 years.
*Title:* New geometric methods for mapping the space of periodic crystals.

2023 – 2025 **Royal Society** International Exchanges with Nicholas Kotov (U Michigan).
*Title:* Geometric invariants for interactions of proteins with nanoparticles.

2022 – 2025 **EPSRC New Horizons** grant (£250K), PI with a postdoc for 20 months.
*Title:* Inverse design of periodic crystals (ref EP/X018474/1).

2021 – 2023 **RAEng Industry Fellowship** (£220K) covering a teaching replacement, the Cambridge Crystallographic Data Centre contributed £60K for a postdoc.

2018 – 2023 **EPSRC £3.5M grant** with Oxford and Swansea, lead co-I at Liverpool with the budget £715K. *Title:* Application-driven Topological Data Analysis.

2017 – 2019 **Royal Society** International Exchanges with H. Edelsbrunner (IST Austria).
*Title:* Topological Data Analysis for a faster discovery of materials.

2011 – 2013 **EPSRC first grant** (£125K) with a postdoctoral assistant for 14 months.
*Title:* Persistent topological structures in noisy images (ref EP/I030328/1).

2005 – 2007 **Marie Curie International Incoming Fellowship** (€142K), Liverpool.

2003 – 2004 Postdoctoral Fellowship by the Council of Burgundy (€22K), France.

2001 – 2003 **INTAS PhD Fellowship** (€10K), Moscow State University.

**Talks at international conferences** since 2019

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| January 2025 | Joint Mathematics Meetings, Seattle, US (4 talks, 105 min in total) |
| October 2024 | SIAM Mathematics of Data Science, Atlanta, US (2-hour tutorial) |
| September 2024 | Computational Persistence (ComPer), Graz, Austria (20 min) |
| July 2024 | Geometric Data Science mini-symposium at 9ECM, Sevilla, Spain (30 min) |
| June 2024 | Biomolecular Topology workshop, Singapore (50-min invited talk) |
| May 2024 | SIAM Mathematical Aspects of Materials Science, Pittsburgh, US (30 min) |
| March 2024 | FANeSy workshop, Santiago, Chile (90-min invited tutorial) |
| January 2024 | Joint Mathematics Meetings, San Francisco, US (5 talks, 130 min in total) |
| August 2023 | International Union of Crystallography Congress, Melbourne (30+30 min) |
| June 2023 | CVPR workshop TAG-PR, Vancouver, Canada (1-hour invited talk) |
| April 2023 | British Crystallographic Association meeting, Sheffield, UK (20 min) |
| January 2023 | Joint Mathematics Meetings, Boston, US (30 min) |
| October 2022 | Fall Workshop in Computational Geometry, Raleigh, US (20 min) |
| October 2022 | International Symposium on Visual Computing, San Diego (20 min) |
| September 2022 | The interdisciplinary world of tangling, Potsdam, Germany (30 min) |
| July 2022 | 32nd International Symposium on Chirality, Chicago, US (30 min) |
| July 2022 | Applied Topology in Frontier Sciences, Singapore (50-min invited talk) |
| July 2022 | Int. Congress of Mathematicians (geometry sec.), Copenhagen (15 min) |
| July 2022 | Applied Topology, Bedlewo Conference Centre, Poland (45-min invited talk) |
| June 2022 | Computational Topology workshop, CGWeek in Berlin (30-min invited talk) |
| October 2021 | Data and Computation for Materials Science and Innovation (20 min) |
| August 2021 | International Union of Crystallography Congress (20+25 min) |
| June 2021 | Online workshop in Geometric Topology (30-min invited talk) |
| May 2021 | The geometry and topology behind fabrics at multiple scales (40 min) |
| April 2021 | Mini-symposium Mathematics for Materials Science at BAMC (20 min) |
| September 2020 | Machine Learning and Dynamical Systems, Fields Institute (30 min) |
| June 2020 | SIAM mini-symposium on Topological Image Analysis, Zoom (25 min) |
| January 2020 | Applied Machine Learning Days, AI & Topology track, EPFL (30 min) |
| November 2019 | Artificial Intelligence for Materials Discovery, Southampton (30 min) |
| August 2019 | Mathematical Crystallography, Vienna, Austria (30 min) |
| July 2019 | Extreme Weather Event Generation, Lorentz centre (45-min invited talk) |
| July 2019 | Accelerating materials discovery, Liverpool, UK (40-min invited talk) |
| April 2019 | BAMC: British Applied Mathematical Colloquium, Bath (20 min) |
| March 2019 | Artificial Intelligence for Materials Discovery, Southampton (30 min) |

**Public engagement**

2019 Science Slam 2nd prize at the European Crystallographic Meeting (Vienna).

2017 Public talk "What can Deep Learning do with Big Data?" at Pint of Science.

**Industrial collaboration**

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| **Impact case study**, since 2021 | 360B+ pairwise comparisons of all 850K+ periodic crystals in the world's largest collection of real materials (Cambridge Structural Database) within one hour on a desktop computer confirmed the Crystal Isometry Principle: any real periodic crystal has a unique geographic-style location in a common Crystal Isometry Space. |
| Cambridge Crystallographic Data Centre since 2018 | RAEng Industrial Fellowship was based on joint papers J34, C20-22 and led to the £60K cash investment for a shared postdoc in addition to the £94K cash to fund three PhD students. |
| Unilever, 2018 – 2024 | Partner in the £3.5M EPSRC grant (2018-2024), which I led in Liverpool, and in the £965K NERC grant (2020-2023), gave £42K cash in 2019 and 2021 for my PhD students, who worked on automatic data processing and plastic waste reduction. |
| Intel Parallel Computing Centre, 2017 – 2020 | Funded my PhD student Grzegorz Muszynzki at Liverpool via the Lawrence Berkeley lab (US). Papers J22-25 and C17 applied Topological Data Analysis to Climate Science for the first time. |
| Microsoft Research, Cambridge, 2014–2016 | C++ programming for a new method of superpixel segmentations [C8, J21] with Andrew Fitzgibbon in the Computer Vision group. |

## Top 3 papers (the full bibliographic details are below)

**[J46] FoCM 2024.** This 59-page paper solved a long-standing problem in metric geometry of periodic lattices, with important applications in materials science, which remained incomplete since the early studies by Lagrange, Gauss, and numerous crystallographers. Atomic vibrations and noise in measurements break all discrete approaches to crystal comparisons and practically motivate studying lattices of rigid crystals in a continuous space. This work analytically defined first continuous distances that satisfy all metric axioms and distinguish all mirror images. As a result, the space of all 2-dimensional lattices under rigid motion has been fully parametrised like a geographic-style map. The extension to dimension 3 is being finalised in arxiv:2201.10543. The follow-up papers [J39, J43] presented the first continuous distributions of lattices in the world's largest database of real materials.

**[C28] CVPR 2023.** This paper with my PhD student, who contributed a software implementation and experiments, solved another long-standing problem in Euclidean geometry, which remained open at least since 1935 (Schoenberg, Annals of Mathematics) when sequences of $m$ ordered points in $\mathbb{R}^n$ were uniquely represented under isometry by a distance matrix or a Gram matrix of scalar products. If these $m$ points are unordered, the brute-force extension to a complete invariant needs $m!$ permutations. In this unordered case,

there were no complete invariants with a Lipschitz continuous metric and *polynomial-time* algorithms (in the number $m$ of points for a fixed dimension $n$) except the case of triangles ($m = 3$) classified by 3 inter-point distances (side-side-side theorem). Even for $m = 4$ points in $\mathbb{R}^2$, there are infinitely many non-isometric clouds of unordered points (with 4 free parameters) that are indistinguishable by all pairwise distances. These counter-examples motivated me to develop much stronger invariants that solved the problem for any $m, n$. The detailed proofs with manual computations are in the extended versions [P7, P8].

**[C27] NeurIPS 2022.** This paper with my PhD student, who contributed a software implementation and experiments, developed a practically sufficient *crystal genome*, which was targeted by the $250M+ Materials Genome Initiative in the US without much progress. Theorem 4.4 proved that a new isometry invariant PDD (Pointwise Distance Distribution) of any generic periodic set $S \subset \mathbb{R}^n$ can be inverted back to $S$. This inverse design justified the *Crystal Isometry Principle* saying that any real periodic crystal is uniquely determined by a precise enough geometry of atomic centres without chemical elements, experimentally checked on the world's largest materials databases within minutes on a desktop, see [P2].

## Preprints (a few more are under a double-blind review and not public yet)

**P10.** J.McManus, V.Kurlin. Computing the bridge length: the key ingredient in a continuous classification of periodic sets, latest pdf, early version in arxiv:2410.23288.

**P9.** D.Widdowson, V.Kurlin. Navigation maps of the material space for self-driving labs of the future, latest pdf, early version in arxiv:2410.13796.

**P8.** V.Kurlin. Simplexwise Distance Distributions for finite spaces with metrics and measures, latest pdf, early version in arxiv:2303.14161.

**P7.** V.Kurlin. The strength of a simplex is the key to a continuous isometry classification of Euclidean clouds of unlabelled points, latest pdf, early version in arxiv:2303.13486.

**P6.** O.Anosova, D.Widdowson, V.Kurlin. Recognition of near-duplicate periodic patterns by continuous metrics with approximation guarantees (under revision in Pattern Recognition), latest pdf, early version in arxiv:2205.15298.

**P5.** V.Kurlin. Complete and continuous invariants of 1-periodic sequences in polynomial time, latest pdf, early version in arxiv:2205.04388.

**P4.** V.Kurlin. A complete isometry classification of 3-dimensional lattices, latest pdf, early version in arxiv:2201.10543.

**P3.** M.Bright, A.Cooper, V.Kurlin. Welcome to a continuous world of 3-dimensional lattices, latest pdf, early version in arxiv:2109.11538.

**P2.** D.Widdowson, V.Kurlin. Pointwise Distance Distributions for detecting near-duplicates in large materials databases, latest pdf (a substantially extended version of C27), early draft in arxiv:2108.04798.

**P1.** O.Anosova, V.Kurlin. Introduction to Periodic Geometry and Topology. The early draft from arxiv:2103.02749 will become a book "Geometric Data Science" in 2025.

## **Peer-reviewed journal articles** (≈2000 citations on Google Scholar)

The key papers developing a new area of Geometric Data Science for chemistry and crystallography are J49-J53, J46, J47, J43, J41, J39, J34, J35, J31, C27-C29. The single-authored papers are P7, P8, P4, P5, J46, J47, J20, J19, J16, J11, J7-J9, J1-J5, C1.

### Two journal papers in 2025

**J53.** A.Wlodawer, Z.Dauter, P.Rubach, W.Minor, M.Jaskolski, W.Jeffcott, Z.Jiang, O.Anosova, V.Kurlin. Duplicate entries in the Protein Data Bank: how to detect and handle them. Acta Crystallographica D, v.81 (4), p.170-180, 2025.

**J52.** O.Anosova, A.Gorelov, W.Jeffcott, Z.Jiang, V.Kurlin. A complete and bi-continuous invariant of protein backbones under rigid motion. MATCH Communications in Mathematical and in Computer Chemistry, v.94 (1), p.97-134, 2025.

### Eight journal papers in 2024

**J51.** D.Widdowson, V.Kurlin. Continuous invariant-based maps of the Cambridge Structural Database. Crystal Growth and Design, v.24(13), p.5627–5636, 2024, extended version (35 pages) available at https://kurlin.org/research-papers.php#CGD2024.

**J50.** O.Anosova, V.Kurlin, M.Senechal. The importance of definitions in crystallography. IUCrJ, v.11(4), p.453-463, 2024, doi:10.1107/S2052252524004056.

**J49.** P.Smith, V.Kurlin. Generic families of finite metric spaces with identical or trivial 1-dimensional persistence. Journal of Applied and Computational Topology (2024), doi:10.1007/s41468-024-00177-6.

**J48.** J.Balasingham, V.Zamaraev, V.Kurlin. Accelerating Material Property Prediction using Generically Complete Isometry Invariants. Scientific Reports, v.14, 10132 (2024).

**J47.** V.Kurlin. Polynomial-time algorithms for continuous metrics on atomic clouds of unordered points. MATCH Communications in Mathematical and in Computer Chemistry, v.91, p.79-108 (2024).

**J46.** V. Kurlin. Mathematics of 2-dimensional lattices. Foundations of Computational Mathematics, v.24, p.805–863 (2024), doi:10.1007/s10208-022-09601-8.

**J45.** J.Balasingham, V.Zamaraev, V.Kurlin. Material Property Prediction using Graphs based on Generically Complete Isometry Invariants. Integrating Materials and Manufacturing Innovation, v.13, p.555-568 (2024). doi:10.1007/s40192-024-00351-9.

**J44.** P.Smith, A.McLauchlin, T.Franklin, P.Yan, E.Cunliffe, T.Hasell, V.Kurlin, C.Kerr, J.Attwood, M.Shaver, T.McDonald. A data-driven analysis of HDPE post-consumer recyclate for sustainable bottle packaging. Resources, Conservation and Recycling, v.205, 107538 (2024).

### Six journal papers in 2023

**J43.** M.Bright, A.Cooper, V.Kurlin. Continuous chiral distances for 2-dimensional lattices. Journal Chirality, v.35 (12), p.920-936 (2023).

**J42.** D.Schwalbe-Koda, D.Widdowson, T.A.Pham, V.Kurlin. Inorganic synthesis-structure maps in zeolites with machine learning and crystallographic distances. Digital Discovery, v.2(6), p.1911-1924 (2023).

**J41.** O.Anosova, V.Kurlin. Density functions of periodic sequences of continuous events. Journal of Mathematical Imaging and Vision, v.65, p.689–701 (2023).

**J40.** M.Torda, J.Goulermas, R.Púček, V.Kurlin. Entropic trust region for densest crystallographic symmetry group packings. SIAM Journal on Scientific Computing, 2023, v.45(4), B493-B522.

**J39.** M. Bright, A. Cooper, V. Kurlin. Geographic-style maps for 2-dimensional lattices. Acta Crystallographica Section A, v.79, p.1-13 (2023).

**J38.** C. Hargreaves et al. A database of experimentally measured lithium solid electrolyte conductivities evaluated with machine learning. npj Computational Materials, 9 (9), 2023, doi:10.1038/s41524-022-00951-z

**Five journal papers in 2022**

**J37.** A. Vriza, I. Sovago, D. Widdowson, P. Wood, V. Kurlin, M. Dyer. Molecular Set Transformer: Attending to the co-crystals in the Cambridge Structural Database. Digital Discovery, v.1, p.834-850 (2022).

**J36.** M. Torda, Y. Goulermas, V. Kurlin, G. Day. Densest plane group packings of regular polygons. Physical Review E, 106, 5, 054603 (2022).

**J35.** Q. Zhu, J. Johal, D. Widdowson, Z. Pang, B. Li, C. Kane, V. Kurlin, G. Day, M. Little, A. Cooper. Analogy Powered by Prediction and Structural Invariants: Computationally-Led Discovery of a Mesoporous Hydrogen-Bonded Organic Cage Crystal. J Amer. Chem. Society, 144, 22, 9893–9901 (2022).

**J34.** D. Widdowson, M. Mosca, A. Pulido, V. Kurlin, A. Cooper. Average Minimum Distances of periodic point sets are fundamental invariants for mapping all periodic crystals. MATCH Communications Math. Comp. Chemistry, v.87(3), p.529-559 (2022).

**J33.** M. Bright, O. Anosova, V. Kurlin. A formula for the linking number in terms of isometry invariants of straight line segments. Computational Mathematics and Mathematical Physics, v.62(8), p.1217-1233 (2022).

**Three journal papers in 2021**

**J32.** Y. Elkin, V. Kurlin. Isometry invariant shape recognition of projectively perturbed clouds by the mergegram extending 0D persistence. Mathematics, v.9(17), 2121 (2021).

**J31.** P. Smith, V. Kurlin. Skeletonisation algorithms with guarantees for unorganised point clouds with high levels of noise. Pattern Recognition, v.115, 107902 (2021).

**J30.** K.Vriza, A.Canaj, R.Vismara, L.Cook, T.Manning, M.Gaultois, P.Wood, V.Kurlin, N.Berry, M.Dyer, M.Rosseinsky. One class classification as a practical approach for accelerating $\pi - \pi$ co-crystal discovery. Chemical Science, v.12, p.1702-1719 (2021).

**Four journal papers in 2020**

**J29.** C. Hargreaves, M. Gaultois, V. Kurlin, M. Rosseinsky. The Earth Mover's Distance as a Metric for the Space of Inorganic Compositions. Chemistry of Materials, v. 32 (24), p. 10610-10620 (2020).

**J28.** M. Bright, V. Kurlin. Encoding and Topological Computation on Textile Structures. Computers & Graphics, v. 90 (2020), p. 51-61.

**J27.** M. Mosca, V. Kurlin. Voronoi-based similarity distances between arbitrary crystal lattices. Crystal Research & Technology, 1900197 (2020), extended at arxiv:2002.11165.

**J26.** V. Kurlin, G. Muszynski. Persistence-based resolution-independent meshes of superpixels Pattern Recognition Letters, v. 131 (2020), p. 300-306.

**Three journal papers in 2019**

**J25.** S. Kalisnik, V. Kurlin, D. Lesnik. A Higher-dimensional Homologically Persistent Skeleton. Advances in Applied Mathematics, v.102, p.113-142 (2019).

**J24.** J. Rutz et al. The Atmospheric River Tracking Method Intercomparison Project: Quantifying Uncertainties in Atmospheric River Climatology. Journal Geophysical Research: Atmospheres, v.124(24), 13777-13802 (2019).

**J23.** G. Muszynski, K. Kashinath, V. Kurlin, M. Wehner, Prabhat. Topological Data Analysis and Machine Learning for Recognizing Atmospheric River Patterns in Large Climate Datasets. Geoscientific Model Development, v.12, p.613-628 (2019).

**Earlier journal papers before 2019**

**J22.** C. Shields et al. Atmospheric River Tracking Method Intercomparison Project. Geoscientific Model Development, v.11, p.2455-2474 (2018).

**J21.** J. Forsythe, V. Kurlin. Convex Constrained Meshes for superpixel segmentations of images. Journal of Electronic Imaging v.26(6), 061609 (2017).

**J20.** V. Kurlin. A fast persistence-based segmentation of noisy 2D clouds with provable guarantees, Pattern Recognition Letters, v.83P1, p.3-12 (2016).

**J19.** V. Kurlin. A one-dimensional Homologically Persistent Skeleton of an unstructured point cloud in any metric space. Computer Graphics Forum, v.34(5), p.253-262 (2015).

**J18.** A. Chernov, V. Kurlin. Reconstructing persistent graphs structures from noisy images. Journal Image-A, v.3, no.5, p.19-22 (2013).

**J17.** V. Kurlin, L. Mihaylova. How many wireless sensors are needed to guarantee connectivity of a 1-dimensional network with random inter-node spacings?
Journal of Applied Probability and Statistics, v.8, no.2, p.27–50 (2013).

**J16.** V. Kurlin. Computing braid groups of graphs with applications to robot motion planning. Homology, Homotopy and Applications, v.14, no.1, p.159-180 (2012).

**J15.** T. Fiedler, V. Kurlin. Recognizing trace graphs of closed braids.
Osaka J. Mathematics, v.47, no.4, p.885–909 (2010).

**J14.** T. Fiedler, V. Kurlin. A one-parameter approach to links in a solid torus.
J. Math. Soc. of Japan, v.62, no.1, p.167–211 (2010). The order of authors is alphabetical. I have learned and applied singularity theory to make all proofs rigorous.

**J13.** T. Fiedler, V. Kurlin. Fiber quadrisecants in knot isotopies.
J. Knot Theory Ramifications, v.17, no.11, p.1415–1428 (2008).

**J12.** C. Kearton, V. Kurlin. All 2-dimensional links live inside a universal 3-dimensional polyhedron. Algebraic and Geometric Topology, v.8, no.3, p.1223–1247 (2008).

**J11.** V. Kurlin. Gauss paragraphs of classical links and a characterization of virtual link groups. Math. Proc. Camb. Phil. Soc., v.145, no.1, p.129–140 (2008).

**J10.** V. Kurlin, D. Lines. Peripherally specified homomorphs of link groups.
J. Knot Theory Ramifications, v.16, no.6, p.719–740 (2007).

**J9.** V. Kurlin. The Baker-Campbell-Hausdorff formula in the free metabelian Lie algebra.
J. Lie Theory, v.17, no.3, p.525–538 (2007).

**J8.** V. Kurlin. Three-page encoding and complexity theory for spatial graphs.
J. Knot Theory Ramifications, v.16, no.1, p.59–102 (2007).

**J7.** V. Kurlin. Compressed Drinfeld associators. J. Algebra, v.292, p.184–242 (2005).

**J6.** V. Kurlin, V. Vershinin. Three-page embeddings of singular knots.
Functional Analysis and Its Applications, v.38, no.1, p.14–27 (2004).

**J5.** V. Kurlin. Basic embeddings of graphs and Dynnikov's method of 3-page embeddings.
Russian Mathematical Surveys, v.58, no.2, p.163–164 (2003).

**J4.** V. Kurlin. Three-page Dynnikov's diagrams of spatial 3-valent graphs.
Functional Analysis and Its Applications v.35, no.3, p.230–233 (2001).

**J3.** V. Kurlin. Basic embeddings into a product of graphs.
Topology and Its Applications, v.102, p.113–137 (2000).

**J2.** V. Kurlin. Reduction of framed links to ordinary links.
Russian Mathematical Surveys, v.54, p.845–846 (1999).

**J1.** V. Kurlin. Invariants of colour links.
Moscow University Mathematical Bulletin, v.54, p.42–44 (1999).

**Peer-reviewed proceedings** or book chapters

**Two conference papers in 2023**

**C29.** Yury Elkin, Vitaliy Kurlin. A new near-linear time algorithm for k-nearest neighbor search using a compressed cover tree. Proceedings of ICML 2023 (International Conference on Machine Learning), p. 9267-9311.

**C28.** D.Widdowson, V.Kurlin. Recognizing rigid patterns of unlabeled point clouds by complete and continuous isometry invariants with no false negatives and no false positives. Proceedings of CVPR 2023 (Computer Vision and Pattern Recognition), 1275-1284.

**Six conference papers in 2022**

**C27.** D. Widdowson, V. Kurlin. Resolving the data ambiguity for periodic crystals. Advances in Neural Information Processing Systems (NeurIPS 2022), v.35, 24625-24638.

**C26.** P. Smith, V. Kurlin. A practical algorithm for degree-k Voronoi domains of three-dimensional periodic point sets. Lecture Notes in Computer Science (Proceedings of ISVC 2022), v.13599, p.377-391.

**C25.** O. Anosova, V. Kurlin. Density functions of periodic sequences. Proceedings of Discrete Geometry and Mathematical Morphology 2022, Lecture Notes in Computer Science, v.13493, p.395-408.

**C24.** Y. Elkin, V. Kurlin. Counterexamples expose gaps in the proof of time complexity for cover trees introduced in 2006 (9 pages). Proceedings of TopoInVis 2022.

**C23.** G. Muszynski, V. Kurlin, D. Morozov, M. Wehner, K. Kashinath, P. Ram. Topological Methods for Pattern Detection in Climate Data. Big Data Analytics in Earth, Atmospheric and Ocean Sciences, p. 227-242, Wiley.

**C22.** J. Ropers, M. Mosca, O. Anosova, V. Kurlin, A. Cooper. Fast predictions of lattice energies by continuous isometry invariants of crystal structures (15 pages). Proceedings of DAMDID: Data Analytics and Management in Data Intensive Domains, p. 178-192.

**Two conference papers in 2021**

**C21.** O. Anosova, V. Kurlin. An isometry classification of periodic point sets. Proceedings of Discrete Geometry and Mathematical Morphology 2021, Lecture Notes in Computer Science, v.12708, p. 229-241.

**C20.** H.Edelsbrunner, T.Heiss, V.Kurlin, P.Smith, M.Wintraecken. The density fingerprint of a periodic point set, 16 pages. Symposium Computational Geometry 2021.

**Five conference papers in 2020**

**C19.** M. Bright, O. Anosova, V. Kurlin. A proof of the invariant-based formula for the linking number and its asymptotic behaviour. Procedings of NumGrid 2020 (Numerical Geometry, Grid Generation and Scientific Computing). Springer Lecture Notes in Computational Science and Engineering, v.143, p.37-60.

**C18.** Y. Elkin, V. Kurlin The mergegram of a dendrogram and its stability. Proceedings of MFCS 2020 (Mathematical Foundations of Computer Science).

**C17.** G. Muszynsky, Prabhat, J. Balewskiy, K. Kashinathy, M. Wehner, V. Kurlin. Atmospheric Blocking Pattern Recognition in Global Climate Model Simulation Data. Proceedings of ICPR 2020 (International Conference on Pattern Recognition).

**C16.** T. Welsch, V. Kurlin. Synthesis through Unification Genetic Programming. Proceedings of GECCO 2020 (Genetic and Evolutionary Computation Conference).

**C15.** A. Siddiqui, V. Kurlin. Polygonal Meshes of Noisy Images based on a new Thinning Algorithm with Theoretical Guarantees. Proceedings of VISAPP 2020 (International Conference on Computer Vision Theory and Applications.

**Three conference papers in 2019**

**C14.** P. Smith, V. Kurlin. Resolution-independent meshes of superpixels. Advances in Visual Computing (Proceedings of International Symposium on Visual Computing 2019), v. 11844, p. 194-205

**C13.** N. Ban, W. Yamazaki, V. Kurlin. Development of a Reconstruction Method for Major Vortex Structure around Tandem Flapping Wing Object via Vortex Trajectory Method. American Institute of Aeronautics and Astronautics SciTech Forum (2019).

**C12.** V. Kurlin, G. Muszynski. A persistence-based approach to automatic detection of line segments in images. Proceedings of CTIC 2019 (Computational Topology in Image Context), LNCS, v. 11382 (2019), p. 137-150.

**Earlier conference papers before 2019**

**C11.** G. Muszynski, K. Kashinath, V. Kurlin, M. Wehner, Prabhat. Towards a topological pattern detection in fluid and climate simulation data. Proc. Climate Informatics 2018.

**C10.** V. Kurlin, D. Harvey. Superpixels Optimized by Color and Shape (SOCS). Proceedings of EMMCVPR 2017, LNCS, v. 10746, p. 297-311.

**C9.** V. Kurlin. Computing invariants of knotted graphs given by sequences of points in 3D. In *Topological Methods in Data Analysis and Visualization IV*, Springer series MathVis: Mathematics and Visualization (2017), p.349-363 (post-proceedings of TopoInVis 2015).

**C8.** J. Forsythe, V. Kurlin, A. Fitzgibbon. *Convex Constrained Meshes of superpixels without small angles.* Proceedings of ISVC 2016: International Symposium on Visual Computing, Lecture Notes in Computer Science, v. 10072 (2016), p. 223-233.

**C7.** V. Kurlin, C. Smithers. A linear time algorithm for embedding arbitrary knotted graphs into a 3-page book. In *Computer Vision, Imaging and Computer Graphics Theory and Applications.* Springer series CCIS: Communications in Computer and Information Science (2016), p. 99-122 (extended from proceedings paper [C4] in IVAPP 2015).

**C6.** V. Kurlin. A Homologically Persistent Skeleton is a fast and robust descriptor of interest points in 2D images. Lecture Notes in Computer Science, v. 9256 (2015), p. 606-617 (Proceedings of CAIP 2015: Computer Analysis of Images and Patterns).

**C5.** H. Edelsbrunner, M. Iglesias-Ham, V. Kurlin. Relaxed disk packing. Proceedings of CCCG 2015: Canadian Conference on Computational Geometry, p. 128–135.

**C4.** V. Kurlin. A linear time algorithm for visualizing knotted structures in 3 pages. Proceedings of IVAPP 2015: Information Visualization Theory & Applications, p.5-16.

**C3.** V. Kurlin, M. Safi-Samghabadi. Computing a skeleton of the configuration space of 2 round robots on a metric graph. Proceedings of ICRoM 2014: IEEE International Conference on Robotics and Mechatronics, p. 723-729.

**C2.** V. Kurlin. Auto-completion of contours in sketches, maps and sparse 2D images. Proceedings of CTIC (Computational Topology in Image Context) at SYNASC 2014 (Symposium on Symbolic & Numeric Algorithms for Scientific Computing), p. 594-601.

**C1.** V. Kurlin. A fast and robust algorithm to count topologically persistent holes in noisy clouds. Proceedings of CVPR 2014: Computer Vision Pattern Recognition, p. 1458-1463.

## Diversity statement (actions on equality, diversity, inclusivity, and accessibility).

Our Data Science group welcomes diverse PhD students and postdoctoral fellows of different genders and cultural backgrounds. If we also count MSc students and interns who co-authored peer-reviewed publications, the group included nationals from 10 countries (UK, USA, Poland, Finland, Italy, Greece, Russia, India, Japan, China). We continuously learn how to best cultivate a climate of respect and courtesy to develop individual potential of every member. Prior to the covid pandemic, the whole group regularly went for lunch before our weekly seminar, which became online in March 2020. Since 2021, we have organised several group walks including family members and partners of different races.

Since 2017 I have led the network Applied Geometry and Topology funded by the London Mathematical Society (LMS), so we strive to uphold all principles on Equality, Diversity, and Inclusion recommended by the LMS. In particular, we invite female speakers and keep our meetings open to all. In the same spirit, I initiated the MIF++ seminar and annual conference MACSMIN, which is co-organised by all group members and featured since 2020 diverse speakers across the world, including females from Iran, Uruguay, Mexico, Japan, Australia, Russia, Canada, and USA. My latest PhD student was hired via shortlisting that hid all names and protective characteristics such as gender, race, etc. As a member of the management team of the CDT in Digital and Automated Materials Chemistry, I support hiring PhD students and other colleagues only by professional skills irrespective of backgrounds. As a co-I in the AI for Chemistry hub, I welcomed the decision to review applications for feasibility studies in the anonymous form. As an area chair at the top Computer Science venues NeurIPS and ICML, I agree that double-blind reviews are fairer than traditional single-blind reviews that can often be influenced by authors' names.