

# Bala Krishnamoorthy: Publications

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## PATENTS

Note: BK stands for Bala Krishnamoorthy

1. BK, Muthu Udaiyanathan, and Sandeep Nair. Slot selection for pickup scheduling and order fulfillment. Patent No. US 12,118,604 B2. Issued on October 15, 2024.

## PUBLICATIONS

1. BK and Alex Tropsha. Development of a four-body statistical pseudo-potential to discriminate native from non-native protein conformations. *Bioinformatics*, 19, 12, 2003, 1540–1548. Preprint and code: [bala-krishnamoorthy.github.io/DT/](https://github.com/bala-krishnamoorthy/DT/).
2. BK, J. Scott Provan, and Alex Tropsha. A topological characterization of protein structure. In *Proceedings of the Conference on Data Mining in BioMedicine*, 2004; edited by Panos M. Pardalos, Vladimir Boginski, and Alkis Vazacopoulos, Springer, 2007 (accepted in 2005), ISBN: 0-387-69318-1. Preprint: [bala-krishnamoorthy.github.io/docs/TopoCharProteins.pdf](https://github.com/bala-krishnamoorthy/docs/TopoCharProteins.pdf).
3. Christopher Deutsch and BK. Four-body scoring function for mutagenesis. *Bioinformatics*, 23, 22, 2007, 3009–3015. Preprint, dataset, and code: [bala-krishnamoorthy.github.io/DT/Mutate](https://github.com/bala-krishnamoorthy/DT/Mutate).
4. BK. Bounds on the size of branch-and-bound proofs for integer knapsacks. *Operations Research Letters*, 36, 1, 2008, 19–25. Preprint: [bala-krishnamoorthy.github.io/docs/BBBounds.pdf](https://github.com/bala-krishnamoorthy/docs/BBBounds.pdf).
5. BK and Gábor Pataki. Column basis reduction and decomposable knapsack problems. *Discrete Optimization*, 6, 3, 2009, 242–270. Preprint: [arxiv:0807.1317](https://arxiv.org/abs/0807.1317).
6. Tamal Dey, Anil Hirani, and BK. Optimal homologous cycles, total unimodularity, and linear programming. In *Proceedings of 42nd ACM Annual Symposium on Theory of Computing (STOC) 2010*, 221–230. Preprint: [arxiv:1001.0338](https://arxiv.org/abs/1001.0338).
7. Ye Tian, Christopher Deutsch, and BK. Optimized scoring function for solubility mutagenesis. *Algorithms for Molecular Biology*, 5, 33, 2010. Dataset, code: [bala-krishnamoorthy.github.io/DT/OptSolMut](https://github.com/bala-krishnamoorthy/DT/OptSolMut).
8. Svetlana Lockwood, BK, and Ping Ye. Neighborhood properties are significant determinants of temperature sensitive mutants. *PLoS ONE*, 6, 12, e28507, 2011, [dx.plos.org/10.1371/journal.pone.0028507](https://doi.org/10.1371/journal.pone.0028507).
9. Tamal Dey, Anil Hirani, and BK. Optimal homologous cycles, total unimodularity, and linear programming. In *SIAM Journal on Computing*, 40, 4, 2011, 1026–1040. This is the expanded version, with some new results, of the STOC 2010 paper (listed as paper # 6).
10. Bethany Suderman, BK, and Anita Vasavada. Neck muscle paths and moment arms are significantly affected by wrapping surface parameters. *Computer Methods in Biomechanics and Biomedical Engineering*, 15, 7, 735–744, 2012. Preprint: [bala-krishnamoorthy.github.io/Papers/WrapSurfSensitivity.pdf](https://github.com/bala-krishnamoorthy/Papers/WrapSurfSensitivity.pdf).
11. BK, William Webb, and Nathan Moyer. Lattice-based algorithms for number partitioning in the hard phase. *Discrete Optimization*, 9, 3, 2012, 159–171.
12. Johannes Elferich, Danielle Williamson, BK, and Ujwal Shinde. Propeptides of eukaryotic proteases encode histidines to exploit organelle pH for regulation. *The FASEB Journal*, 27, 8, 2013, 2939–2945.
13. Sharif Ibrahim, BK, and Kevin Vixie. Simplicial flat norm with scale. *Journal of Computational Geometry*, 4, 1, 2013, 133–159. Preprint: [arxiv:1105.5104](https://arxiv.org/abs/1105.5104).
14. Tamal Dey, Anil Hirani, BK, and Gavin Smith. Edge contractions and simplicial homology. Submitted, 2013. Preprint: [arXiv:1304.0664](https://arxiv.org/abs/1304.0664).
15. BK, Brian Bay, and Robert Hart. Bone mineral density and donor age are not predictive of femoral ring allograft bone mechanical strength. *Journal of Orthopaedic Research*, 32, 10, 2014, 1271–1276. Preprint: [bala-krishnamoorthy.github.io/Papers/Allograft.pdf](https://github.com/bala-krishnamoorthy/Papers/Allograft.pdf).
16. Nathan Hamlin, BK, and William Webb. A knapsack-like code using recurrence sequence representations. *Fibonacci Quarterly*, 53, 1, 2015, 24–33. Preprint: [arXiv:1503.04238](https://arxiv.org/abs/1503.04238).
17. Svetlana Lockwood and BK. Topological features in cancer gene expression data. In *Proceedings of the Pacific Symposium on Biocomputing*, 20, 2015, 108–119. Preprint: [arXiv:1410.3198](https://arxiv.org/abs/1410.3198).

18. BK and Gavin Smith. Non total-unimodularity neutralized simplicial complexes. *Discrete Applied Mathematics*, 240, 11, 2018, 44–62 (published online Feb 3, 2016). Preprint: arxiv:1304.4985.
19. Sharif Ibrahim, BK, and Kevin Vixie. Flat Norm Decomposition of Integral Currents. *Journal of Computational Geometry*, 7, 1, 2016, 285–307. Preprint: arXiv:1411.0882.
20. BK. Thinner is not always better: Cascade knapsack problems. *Operations Research Letters*, 45, 1, 77–83, 2017. Preprint and instances: bala-krishnamoorthy.github.io/CKP/.
21. Sabina Blizzard, BK, Matthew Shinseki, Marcel Betsch, and Jung Yoo. The magnitude of angular and translational displacement of dens fractures is dependent on the sagittal alignment of the cervical spine rather than the force of injury. *The Spine Journal*, 17, 12, 1859–1865, 2017. Preprint: bala-krishnamoorthy.github.io/docs/Lordosis.pdf.
22. Philip Behrend and BK. Considerations for waste gasification as an alternative to landfilling in Washington state using decision analysis and optimization. *Sustainable Production and Consumption*, 12, 170–179, 2017. Preprint: bala-krishnamoorthy.github.io/Papers/WasteGasification.pdf.
23. Dayton Opel, Benjamin Rapone, BK, Jung Yoo, and James Meeker. Race and gender influence management of humerus shaft fractures. *Journal of Orthopaedics*, 15, 2, 2018, 540–544. Preprint: bala-krishnamoorthy.github.io/docs/Humerus.pdf.
24. Methun Kamruzzaman, Ananth Kalyanaraman, and BK. Detecting divergent subpopulations in phenomics data using interesting flares. In the Proceedings of the 9th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (BCB '18), 155–164, 2018.
25. Marcel Betsch, Sabina Blizzard, BK, and Jung Yoo. Association between cervical spine degeneration and the presence of dens fractures. *Zeitschrift für Orthopädie und Unfallchirurgie*, 158, 01, 2020, 46–50 (published online Apr 9, 2019). Preprint: bala-krishnamoorthy.github.io/Papers/DensFractures.pdf.
26. Kaniz F. Madhobi, Methun Kamruzzaman, Ananth Kalyanaraman, Eric Lofgren, Rebekah Moehring, and BK. A visual analytics framework for analysis of patient trajectories. In the Proceedings of the 10th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (BCB '19), 2019.
- ⇒ A shorter version of the above paper was accepted to the ACM SIGKDD Workshop titled *epiDAMIK: Epidemiology meets Data Mining and Knowledge discovery*, 2019.
27. Yunfeng Hu, Matthew Hudelson, BK, Altaa Tumurbaatar, and Kevin Vixie. Median Shapes. *Journal of Computational Geometry*, 10, 1, 2019, 322–388. Preprint: arXiv:1802.04968.
28. Methun Kamruzzaman, Ananth Kalyanaraman, BK, Stefan Hey, and Patrick S. Schnable. Hyppo-X: A scalable exploratory framework for analyzing complex phenomics data. *IEEE Transactions on Computational Biology and Bioinformatics*, 18, 4, 2021, 1535–1548 (published online in October, 2019).
29. Ananth Kalyanaraman, Methun Kamruzzaman, and BK. Interesting paths in the mapper complex. *Journal of Computational Geometry*, 10, 1, 2019, 500–531. Preprint: arXiv:1712.10197.
30. Prashant Gupta, BK, and Gregory Dreifus. Continuous toolpath planning in a graphical framework for sparse infill additive manufacturing. *Computer-Aided Design*, 127, 2020, 102880. Issue on papers accepted to Solid and Physical Modeling (SPM 2020). Preprint: arXiv:1908.07452.
31. Enrique Alvarado, Zhu Liu, Michael Servis, BK, and Aurora Clark. A geometric measure theory approach to identify complex structural features of soft matter surfaces. *Journal of Chemical Theory and Computation*, 16, 7, 2020, 4579–4587. Preprint: ChemRxiv:10.26434/chemrxiv.11988048.v1.
32. Prashant Gupta and BK. Euler transformation of polyhedral complexes. *International Journal of Computational Geometry & Applications (IJCGA)*, 30, 03n04, 2020, 183–211. Preprint: arXiv:1812.02412.
33. Yunfeng Hu, Phonemany Ounkham, Ondrej Marsalek, Thomas Markland, BK, and Aurora Clark. Persistent homology metrics reveal quantum fluctuations and reactive atoms in path integral dynamics. *Frontiers in Chemistry*, 9, 2021. Preprint: ChemRxiv:10.26434/chemrxiv.13618922.
34. Joshua Mirth, Yanqin Zhai, Johnathan Bush, Enrique Alvarado, Howie Jordan, Mark Heim, BK, Markus Pflaum, Aurora Clark, Y Z, and Henry Adams. Representations of energy landscapes by sublevelset persistent homology: An example with n-alkanes. *The Journal of Chemical Physics*, 154, 11, 2021, p114114. Preprint: arXiv:2011.00918.

35. Enrique Alvarado, BK, and Kevin Vixie. The maximum distance problem and minimal spanning trees. *International Journal of Analysis and Applications*, 19, 5, 2021, 633–659. Preprint: arXiv:2004.07323.
36. Youjia Zhou, Methun Kamruzzaman, Patrick Schnable, BK, Ananth Kalyanaraman, and Bei Wang. Pheno-Mapper: An interactive toolbox for the visual exploration of phenomics data. In the Proceedings of the 12th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (BCB '21), Article 20, 2021, 1–10. Preprint: arXiv:2106.13397.
37. Prashant Gupta, Yiran Guo, Narasimha Boddeti, and BK. SFCDecomp: Multicriteria optimized tool path planning in 3D printing using space-filling curve based domain decomposition. *International Journal of Computational Geometry & Applications (IJCGA)*, 31, 04, 2021, 193–220. arXiv:2109.01769.
38. Matthew Broussard, BK, David Makin, Dale Willits. Extracting insights on use of force by police in encounters through topological data analysis of body-worn camera video datasets. Submitted, 2021. Preprint: bala-krishnamoorthy.github.io/docs/BWCVideosTDA.pdf.
39. Methun Kamruzzaman, Matthew Bielskas, BK, Achla Marathe, Anil Vullikanti, and Ananth Kalyanaraman. Navigating the COVID-19 data landscape: Automated hypothesis generation using topological data analysis. Submitted, 2021. Preprint: ResearchSquare (DOI: 10.21203/rs.3.rs-470082/v1).
40. Youjia Zhou, Nathaniel Saul, Ilkin Safarli, BK, and Bei Wang. Stitch Fix for Mapper and Topological Gains. *Research In Computational Topology 2*, 2022, 265–294. Preprint: arXiv: 2105.01961.
41. Hung Le, Sushant Kumar, Nathan May, Ernesto Martinez-Baez, Ravishankar Sundararaman, BK, and Aurora Clark. Behavior of linear and nonlinear dimensionality reduction for collective variable identification of small molecule solution-phase reactions. *Journal of Chemical Theory and Computation*, 18, 3, 2022, 1286–1296. Preprint: ChemRXiv.
42. Sejal Welankar, Paola Pesantez-Cabrera, BK, Lynn Mills, Markus Keller, and Ananth Kalyanaraman. Persistent homology to study cold hardiness of grape cultivars. In the Proceedings of the Workshop on AI for Agricultural and Food Systems (AIAFS) at the 37th AAAI Conference on Artificial Intelligence (AAAI-23) (also selected for lightning talk+poster). Preprint: arXiv:2302.05600.
43. Krishnamurthy Dvijotham, BK, Yunqi Luo, and Benjamin Rapone. Robust feasibility of systems of quadratic equations using topological degree theory. *Optimization Letters*, 18, 2024, 591–613 (published online in May 2023). arXiv:1907.12206.
44. Rounak Meyur, Kostiantyn Lyman, BK, and Mahantesh Halappanavar. Structural validation of synthetic power distribution networks using the multiscale flat norm. In Proceedings of the International Conference on Computational Science (ICCS 2023), *Lecture Notes in Computer Science*, vol 10476, 2023, 55–69.
45. David Makin, Guangzhen Wu, Matthew Broussard, and BK. Predicting Police Integrity: An Application of Support Vector Machines (SVM) to The Police Integrity Instrument. *Asian Journal of Criminology*, 19, 2024, 69–93. Preprint: bala-krishnamoorthy.github.io/docs/Integrity.pdf.
46. Matthew Broussard and BK. A tight max-flow min-cut duality theorem for non-linear multicommodity flows. *Journal of Combinatorial Optimization (JoCO)*, 47, 2024, article 54. Preprint: arXiv:2107.04252.
47. Yunqi Luo, Rabayet Sadnan, BK, and Anamika Dubey. Convergence guarantees of a distributed network equivalence algorithm for distribution-OPF. Refereed paper in the 2024 INFORMS Optimization Society Conference (IOS2024). Preprint: arXiv:2210.17465.
48. S M Ferdous, Bhargav Samineni, Mahantesh Halappanavar, and BK. Approximate Bipartite  $b$ -Matching using Multiplicative Auction. Refereed paper in the 2024 INFORMS Optimization Society Conference (IOS2024). arXiv:2403.05781.
49. Nathan May, BK, and Patrick Gambill. A normalized bottleneck distance on persistence diagrams and homology preservation under dimension reduction. *La Matematica*, 3, 2024, 1486–1509. Preprint: arXiv:2306.06727.
50. S M Ferdous, Bhargav Samineni, Alex Pothén, Mahantesh Halappanavar, and BK. Semi-Streaming Algorithms for Weighted  $k$ -Disjoint Matchings. In the Proceedings of the 32nd Annual European Symposium on Algorithms (ESA 2024), *LIPICs*, 308, 2024, 53:1–53:19. arXiv:2311.02073.
51. Fabiana Ferracina, BK, Mahantesh Halappanavar, Shengwei Hu, and Vidyasagar Sathuvalli. Predictive analytics of selections of russet potatoes. In *Crop Science*, 65, e21432, 2025. arXiv:2404.03701.

52. Enrique Alvarado, BK, and Kevin Vixie. Geometry of a Set and its Random Covers. *Moroccan Journal of Pure and Applied Analysis (MJPAA)*, 11, 1, 2025, 1–29. arXiv:2112.14979.
53. Dustin Arendt, Matthew Broussard, BK, Nathaniel Saul, and Amber Thrall. Steinhaus filtration and stable paths in the Mapper. In the Proceedings of the 41st International Symposium on Computational Geometry (SoCG), LIPIcs, 332, 2025, 10:1–10:21. Full version: arXiv:1906.08256.
54. Fabiana Ferracina, Payton Beeler, Mahantesh Halappanavar, BK, Marco Minutoli, and Laura Fierce. Learning to Simulate Aerosol Dynamics with Graph Neural Networks. In *Environmental Science & Technology*, 2, 8, 2025, 1426–1438. arxiv:2409.13861.
55. Kostiantyn Lyman, Rounak Meyur, BK, and Mahantesh Halappanavar. Structural validation of synthetic power distribution networks using the multiscale flat norm. In *International Journal of Computational Geometry & Applications (IJCGA)*, 2025. This is a substantially expanded version of the ICCS 2023 paper (listed as paper # 44). arXiv:2403.12334.
56. Enrique Alvarado, Prashant Gupta, and BK. Box Filtration. In *Journal of Applied and Computational Topology*, 9, 23, 2025. Preprint: arXiv:2404.05859.
57. Viraj Sawant, Kaiyi Wang, Vicky Tong, Zachary Fendler, BK, Seema Gandhi, and Deepak Rajagopal. A new heuristic framework for estimating indirect (Scope 3) emissions of large organizations. In *Nature Scientific Reports*, 15, 36539, 2025.
58. Patrick Gambill, Devesh Jha, BK, Arvind Raghunathan, and William Yerazunis. DamageEst: Accurate Estimation of Damage for Repair using Additive Manufacturing. In the Proceedings of the 36th Annual International Solid Freeform Fabrication Symposium (SFFS), 2025.
59. Jackson Elowitt, Nathan May, Yihui Wei, Enrique Alvarado, BK, and Aurora Clark. Electron Density Transport During Chemical Reactions. To appear in *Journal of Chemical Theory and Computation*, 2025. Preprint: ChemRXiv.
60. BK and Kostiantyn Lyman. Efficient Network Flow Models for Optimal Homology Problems over the Integers. Submitted, 2024 (based on arXiv:2406.19422).
61. BK and Elizabeth Thompson. A Stable Measure for Conditional Periodicity of Time Series using Persistent Homology. Submitted, 2025. Preprint: arXiv:2501.02817.
62. Shishir Lamichhane, Abodh Poudyal, Nicholas Jones, BK, and Anamika Dubey. Scalable Two-Stage Stochastic Optimal Power Flow via Separable Approximation. Submitted, 2025. arXiv:2504.13933.
63. Shishir Lamichhane, Nicholas Jones, BK, and Anamika Dubey. Scalable Stochastic Siting and Sizing of Distributed Generators using Separable Approximation. Submitted, 2025.
64. Elizabeth Thompson, Mary McMillin, Dale Willits, David Makin, Ella Schulz, BK. Does Coding Change What We See? The Influence of Annotation on Perceptions of Police Use of Force. Submitted, 2025. Preprint: crimRxiv.
65. Amber Thrall, Vidya Chhabria, S M Ferdous, Mahantesh Halappanavar, BK. LockRoute: A Spatial Locking Framework for Parallel Global Routing. Submitted, 2025.

#### ABSTRACTS IN MEDICAL CONFERENCES

Note: These abstracts are typically two pages long, and are peer reviewed. A small number of abstracts are elevated to oral presentations (rest are presented as e-posters).

1. BK, Brian Bay, and Robert Hart. Bone mineral density and donor age are not predictive of allograft bone mechanical strength. E-Poster in the Lumbar Spine Research Society (LSRS) Annual Meeting, 2013.
2. BK, Brian Bay, and Robert Hart. Bone mineral density and donor age are not predictive of allograft bone mechanical strength. E-Poster in the North American Spine Society (NASS) Annual Meeting, 2013.
3. Jung Yoo, Matthew Shinseki, Sabina Blizzard, Marcel Betsch, BK, and Jayme Hiratzka. Why Do Dens Fractures Occur in the Elderly and What Determines the Magnitude of Fracture Angulation and Displacement? Oral presentation in the Korean American Spine Society (KASS) Annual Meeting, 2015.

4. Jung Yoo, Sabina Blizzard, Natalie Zusman, Matthew Shinseki, Marcel Betsch, and BK. Dens Fractures Displacement Is Dependent On The Sagittal Alignment Of The Subaxial Cervical Spine Rather Than The Force Of Injury. Oral presentation in the Cervical Spine Research Society (CSRS) Annual Meeting, 2015.
5. Dayton Opel, Benjamin Rapone, BK, Jung Yoo, James Meeker. Race and Gender Influence Management of Humerus Shaft Fractures. Podium presentation at the 80th Annual Meeting of the Western Orthopaedic Association, 2016.
6. Dayton Opel, Benjamin Rapone, BK, Jung Yoo, James Meeker. Race and Gender Influence Management of Humerus Shaft Fractures. Poster at 104th Annual Meeting of the Clinical Orthopaedic Society, 2016.

#### **POSTERS IN CONFERENCES**

Note: A 1–2 page abstract is reviewed as part of the selection process. These abstracts are published as part of the proceedings of the conference.

1. Methun Kamruzzaman, Ananth Kalyanaraman, and BK. Characterizing the Role of Environment on Phenotypic Traits using Topological Data Analysis. In the 7th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM BCB 2016).
2. Gregory Dreifus, Ben Rapone, John Bowers, Xiang Chen, A. John Hart, and BK. A Framework for Tool Path Optimization in Fused Filament Fabrication. In the ACM Symposium on Computational Fabrication, June 2017.
3. Ananth Kalyanaraman, Methun Kamruzzaman, and BK. Interesting paths in the Mapper. In Algebraic Topology: Methods, Computation and Science (ATMCS8), June 2018.
4. Liya Boukhbinder, Lauren McDermott, BK, and Sukanta Bose. UMAP-Based Convex Hull Separation of GW Signals vs Glitches. In the Gravitational Wave Physics and Astronomy Workshop 2025 (GWPAW).

#### **YOUNG RESEARCHERS FORUM (YRF) SUBMISSIONS**

Note: Students present their work as talks in the YRF held as part of the International Symposium on Computational Geometry (SoCG). A short abstract is reviewed as part of the selection process, but not formally published. Student presenter is marked with an asterisk (\*).

1. Tamal Dey, Anil Hirani, BK, and Gavin Smith\*. Edge contractions and the optimal homologous chain problem. 2012.
2. Sharif Ibrahim\*, BK, and Kevin Vixie. Multiscale simplicial flat norm. 2012.
3. BK and Gavin Smith\*. Non total-unimodularity neutralized simplicial complexes. 2013.
4. BK, Nathaniel Saul\*, and Bei Wang. Stitch fix for mapper. 2018.
5. Dustin Arendt, BK, and Nathaniel Saul\*. Jaccard filtration and stable paths in the Mapper. 2019.