David E. Bernal Neira

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Summary

Principal investigator of the **S**ystems **E**ngineering via **C**lassical and **Qu**antum **O**ptimization for **I**ndustrial **A**pplications (SECQUOIA) research group at Purdue University and Assistant Professor at the Davidson School of Chemical Engineering at that university. Adjunct Professor of Operations Management and Quantum Computing at the Tepper School of Business of Carnegie Mellon University.

Research interests

- Special interest in optimization applications in Chemical Engineering and Process Systems Engineering such as Process Intensification and Energy Systems Optimal Process Synthesis, Design, Operation, and Control.
- Quantum Algorithms for Combinatorial Optimization, with emphasis in Chemical Engineering applications.
- Development and evaluation of novel hardware algorithms for optimization and chemistry.
- Theory and applications of Decision-making Optimization, Machine Learning, and Artificial Intelligence.
- Discrete-Continuous Nonlinear Optimization Solution Algorithms, Theory, and Software.

Education

Carnegie Mellon University — Pittsburgh, PA, USA
Ph.D. in Chemical Engineering, Advisor: Prof. Ignacio E. Grossmann, GPA: 3.92/4.00 — 01/2017–05/2021

Universidad de los Andes — Bogotá, Colombia
B.S. in Physics, GPA: 4.62/5.00 — 01/2011–03/2018

M.S. in Chemical Engineering, GPA: 4.73/5.00 — 08/2014–10/2016

B.S. in Chemical Engineering with Honors - Cum Laude, GPA: 4.62/5.00 — 08/2010–10/2014

Experience

Purdue University – Davidson School of Chemical Engineering — West Lafayette, IN, USA
Assistant Professor — 08/2023-Current

– Principal investigator of the **S**ystems **E**ngineering via **C**lassical and **Qu**antum **O**ptimization for **I**ndustrial **A**pplications (SECQUOIA) research group

NASA - Universities Space Research Association (USRA) — Mountain View, CA, USA
Visiting Scientist at USRA Research Institute of Advanced Computer Science (RIACS) — 08/2023-08/2024

Visiting Scientist at NASA Quantum and Artificial Intelligence Laboratory (QuAIL) — 08/2023-06/2024

Research Scientist at NASA QuAIL — 06/2021-07/2023

Associate Scientist at USRA RIACS — 06/2021-07/2023

– Study and design of optimization algorithms that exploit quantum computing for science and engineering

Ph.D. Intern as part of Feynman Quantum Academy NASA QuAIL and USRA RIACS — 05/2019-08/2019

– Development and Implementation of Computational Algebraic Geometry and Integer Programming based compiler for Quantum Annealing problem embedding

Carnegie Mellon University – Tepper School of Business Pittsburgh, PA, USA
Adjunct Professor of Operations Management and Quantum Computing 08/2023-Current

- Lecturer of the Quantum Integer Programming and Machine Learning course offered by Electrical and Computers Engineering and the Tepper School of Business

Carnegie Mellon University – Department of Chemical Engineering Pittsburgh, PA, USA
Visiting Research Scholar 06/2021-08/2022

- Management of Grossmann Research Group meetings
- Maintenance of Mixed-Integer Nonlinear and Generalized Disjunctive Programming Library minlp.org

Ph.D. Student 01/2017-05/2021

- Algorithm development and study for optimization problems with application in chemical, process, and energy systems engineering
- Algorithm development for Mixed-Integer Nonlinear Programming and Generalized Disjunctive Programming
- Study of short-term quantum computing techniques for combinatorial optimization

Visiting Research Scholar 05/2015-08/2015

- Implementation of Mixed-Integer Nonlinear Programming (MINLP) heuristic algorithms in solver DICOPT

ExxonMobil Engineering and Research Company Clinton, NJ, USA
Ph.D. Intern at Corporate Strategic Research Division 05/2020-08/2020

- Evaluation of quantum computing for solving optimization problems relevant to logistics in oil & gas

Ph.D. Intern at the Process Technology Department 05/2018-08/2018

- Development, implementation, and deployment of a combined heat and power plant with carbon capture technologies optimal operation model

Universidad de los Andes – Department of Chemical Engineering Bogotá, Colombia
Graduate Teaching and Research Assistant 08/2014-07/2016

- Researcher in the Process and Products Design Group and the Processes Optimization Group

Bayer Technology Services Leverkusen, Germany
Undergraduate Intern 02/2013-07/2013

- Modeling and automatic implementation of dynamic flooding in distillation columns, and thermodynamic and electrolytic effects in HCl water absorption for acid absorption columns simulation

Awards and Honors

- Arab-American Frontiers Fellowship 2024
National Academies of Science, Engineering, and Medicine
- Best talk award at the Quantum Computing Applications in Chemical and Biochemical Engineering Workshop 2022
American Institute of Chemical Engineers and Technical University of Denmark
- Finalist for AIChE CAST Directors' Student Presentation Awards 2020
Computing & Systems Technology Division (CAST) - American Institute of Chemical Engineers
- Mark Dennis Karl Outstanding Teaching Assistant Award 2019
Chemical Engineering Department - Carnegie Mellon University
- Cum Laude in Chemical Engineering 2014
Universidad de los Andes
- Alberto Magno Scholarship 2010-2014
Universidad de los Andes
- Valedictorian 2009
Gimnasio Británico
- First Place National Physics Olympiads Superior Level 2007
Colombian Mathematics and Physics Olympiads

Teaching

Purdue University West Lafayette, IN, USA
Course Instructor at the Davidson School of Chemical Engineering Fall 2023

- CHE 456 Process Dynamics and Control undergraduate course

Carnegie Mellon University Pittsburgh, PA, USA
Lecturer in the Tepper School of Business and Electrical and Computers Engineering Fall 2023

- 47-779 / 47-785 Quantum Integer Programming and Quantum Machine Learning graduate course

Invited Lecturer in the Tepper School of Business and Electrical and Computers Engineering Fall 2022

- 47-779 / 47-785 Quantum Integer Programming and Quantum Machine Learning graduate course

Course Instructor in the Tepper School of Business and Electrical and Computers Engineering Fall 2021

- 47-779 / 47-785 Quantum Integer Programming and Quantum Machine Learning graduate course

Course Instructor in the Tepper School of Business Fall 2020

- 47-779 Quantum Integer Programming graduate course

Graduate Teaching Assistant in the Chemical Engineering Department

- 06-421 Chemical Process Systems Design undergraduate course. Fall 2017, Fall 2018
  - *Mark Dennis Karl Outstanding Teaching Assistant Award*
- 06-720 Advanced Process Systems Engineering graduate course Spring 2018
- 06-805 Special Topics in Chemical Engineering – Disjunctive Programming graduate course Spring 2018

Universidad de los Andes Bogotá, Colombia
Graduate Recitation Leader in the Chemical Engineering Department 2014–2016

- IQUI3040 Chemical Process Optimization 2015-2016
- IQUI2021 Phase and Chemical Equilibrium 2014

Undergraduate Teaching Assistant and Grader 2010–2014

- IQUI3001 Separation Processes and IQUI3040 Chemical Process Optimization in the Chemical Engineering Department
- FISI1518 Physics 1, FISI1528 Physics 2, and FISI2540 Thermodynamics in the Physics Department
- MATE1203 Differential Calculus and MATE2301 Differential Equations in the Mathematics Department

Teaching-related Training

- Future Faculty Program - CMU Eberly Center for Teaching Excellence and Educational Innovation 2019–2022
- Teaching Effectiveness Colloquium - Institute for Operations Research and Management Science 2020

Mentoring

Purdue University West Lafayette, IN, USA
Davidson School of Chemical Engineering 2023-Current

- Yirang Park - Ph.D. Candidate 2023-Current
- Anurag Ramesh - Ph.D. Candidate 2023-Current
- Albert Lee - Ph.D. Candidate 2022-Current
- Hamta Bardool - Postdoctoral Associate 2024-Current
- Carolina Tristán - Postdoctoral Associate 2024-Current
- Amandeep Singh Bhatia - Postdoctoral Associate 2023-2024

- Zedong Peng - Postdoctoral Associate 2023-2024
- Juan Sebastián Rodríguez - Visiting Research Scholar Spring 2024
- Andrés Cabeza - Visiting Research Scholar Fall 2023, Spring 2024
- Pedro Maciel Xavier - Visiting Research Scholar Fall 2023
- Abigail Delaney - Undergraduate Researcher Fall 2024
- Lukas Peng - Undergraduate Researcher Fall 2024
- Dale Stager - Undergraduate Researcher Fall 2024
- Keegan Duffin - Undergraduate Researcher Fall 2024
- Dhruv Mendpara - Undergraduate Researcher Fall 2024
- Benjamin Murray - Undergraduate Researcher Spring 2024-Fall 2024
- Sergio Barrios - Undergraduate Researcher Fall 2023

NASA - Universities Space Research Association Mountain View, CA, USA
Feynmann Quantum Academy 2021-2024

- Farshud Sorourifar - Ph.D. in Chemical Engineering at Ohio State University
- Robin Brown - Ph.D. in Computational and Mathematical Engineering at Stanford University
- Phillip Kerger - Ph.D. in Applied Mathematics and Statistics at Johns Hopkins University
- Pratik Sathe - Ph.D. in Physics at the University of California in Los Angeles
- Dan Zhao - M.Sc. in Computer Science at the New York University
- Diana Chamaki - B.Sc. in Physics at the University of California in Berkeley
- Christopher Um - B.Sc. in Physics at Cornell University

Carnegie Mellon University Pittsburgh, PA, USA
Chemical Engineering M.Sc. students Research 2018-2020

- Yunshan Liu
- Haokun Yang

Chemical Engineering undergraduate students Honors Research 2018-2020

- Felicity Gong
- Rahul Joglekar
- Saeed Syed
- Zhifei Yuliu

Universidad de los Andes Bogotá, Colombia
Chemical Engineering undergraduate students Thesis 2015-2016

- Paola Cristancho
- Hugo Cuellar

Ph.D. Thesis committee member

- Carolina Tristán - Chemical Engineering, Universidad de Santander, Cantabria, Spain. Title: Advancing sustainability in the water-energy nexus. Optimization of reverse electrodialysis energy recovery from salinity gradients
- Phillip Kerger - Applied Mathematics and Statistics, Johns Hopkins University, Baltimore, MD, USA. Title: Topics in Classical and Quantum Optimization: Complexity and Algorithms
- Rodolfo Quintero - Industrial and Systems Engineering, Lehigh University, Bethlehem, PA, USA. Title: Exact Penalization, Lagrangian Relaxation, and Applications to Quantum Computing
- Hsuan-Hao Hsu - Chemical Engineering, Purdue University, West Lafayette, IN, USA. Title: Computational Reaction Discovery Algorithms for Open-Shell and Ionic Organic Species

Other

Master students advised externally

- Pedro Maciel Xavier, Systems and Computing Engineering, Federal University of Rio de Janeiro, Brazil 2024
- Pedro da Silveira Carvalho Ripper, Electrical Engineering, Pontifical Catholic University of Rio de Janeiro, Brazil 2024

Students Awards and Honors

• Andres Cabeza - Best presentation in the AIChE LatinX Virtual Meeting 2023
American Institute of Chemical Engineers LatinX Division

• Haokun Yang - Best submission in the Refining and Petrochemical Plant Modeling and Operations Improvement Session: "Integration of Crude-Oil Scheduling and Refinery Planning By Lagrangean Decomposition Approach" 2018
AIChE Annual Meeting

Short Courses and Workshops Taught

- Invited Summer School: Optimization in Biorefineries - Universidad Nacional, Bogota, Colombia 07/2024
- Workshop: Practical workshop on Quantum Computing for Optimization for Process Systems Engineering - PSE/ESCAPE34, Florence, Italy 06/2024
- Master Class: Quantum Computing for CP, AI, and OR, and vice-versa: Quantum-Classical Hybrid Methods for Optimization - CPAIOR, Uppsala, Sweden 05/2024
- Invited Workshop: Quantum Integer Programming - Key Laboratory of Data Analytics and Optimization for Smart Industry, Northeastern University, Shenyang, China 04/2024
- Invited Workshop: Quantum Integer Programming - Key Laboratory of Data Analytics and Optimization for Smart Industry, Northeastern University, Shenyang, China 04/2024
- Invited Short Course: Quantum Computing in Optimization - Electrical Engineering and Computer Science, Khalifa University, Abu Dhabi, United Arab Emirates 03/2024
- Invited Short Course Lectures: 2023 Gene Golub SIAM Summer School on Quantum Computing and Optimization - Lehigh University, Bethlehem, PA, USA 08/2023
- Short Course: Mixed-Integer and Disjunctive Optimization Theory, Software, and Algorithms - Institute of Industrial & Systems Engineering, Northeastern University, Shenyang, China 04/2019
- Software Workshop: Mathematical Programming in Python/Pyomo - Instituto de Desarrollo y Diseño INGAR CONICET-Universidad Tecnológica Nacional, Santa Fé, Argentina 08/2018

Journal Publications

[J1] **D. E. Bernal** and I. E. Grossmann, "Convex mixed-integer nonlinear programs derived from generalized disjunctive programming using cones", *Computational Optimization and Applications*, pp. 1–62, 2024. DOI: 10.1007/s10589-024-00557-9.

[J2] **D. E. Bernal**, C. D. Laird, L. R. Lueg, S. M. Harwood, D. Trenev, and D. Venturelli, "Utilizing modern computer architectures to solve mathematical optimization problems: A survey", *Computers & Chemical Engineering*, p. 108 627, 2024. DOI: 10.1016/j.compchemeng.2024.108627.

[J3] R. Brown, **D. E. Bernal**, D. Venturelli, and M. Pavone, "Copositive programming for mixed-binary quadratic optimization via Ising solvers", *SIAM Journal on Optimization*, vol. 34, no. 2, pp. 1455–1489, 2024. DOI: 10.1137/22M1514581.

[J4] T. Lubinski, C. Coffrin, C. McGeoch, P. Sathe, J. Apanavicius, and **D. E. Bernal**, "Optimization applications as quantum performance benchmarks", *ACM Transactions on Quantum Computing*, 2024. DOI: 10.1145/3678184.

[J5] E. G. Rieffel, A. A. Asanjan, M. S. Alam, N. Anand, **D. E. Bernal**, S. Block, L. T. Brady, S. Cotton, Z. G. Izquierdo, S. Grabbe, *et al.*, "Assessing and advancing the potential of quantum computing: A NASA case study", *Future Generation Computer Systems*, vol. 160, pp. 598–618, 2024, **Editor's choice paper**. DOI: 10.1016/j.future.2024.06.012.

[J6] J. Wang, Z. Peng, R. Hughes, D. Bhattacharyya, **D. E. Bernal**, and A. W. Dowling, "Measure This, Not That: Optimizing the Cost and Model-Based Information Content of Measurements", *Computers & Chemical Engineering*, vol. 189, p. 108 786, 2024. DOI: 10.1016/j.compchemeng.2024.108786.

[J7] P. Kerger, **D. E. Bernal**, Z. Gonzalez Izquierdo, and E. G. Rieffel, "Mind the $\tilde{O}$: Asymptotically Better, but Still Impractical, Quantum Distributed Algorithms", *Algorithms*, vol. 16, no. 7, 2023, ISSN: 1999-4893. DOI: 10.3390/a16070332.

[J8] L. Su, **D. E. Bernal**, I. E. Grossmann, and L. Tang, "Modeling for integrated refinery planning with crude-oil scheduling", *Chemical Engineering Research and Design*, vol. 192, pp. 141–157, 2023. DOI: 10.1016/j.cherd.2023.02.008.

[J9] **D. E. Bernal**, "Coherent simulation with thousands of qubits", *Nature Physics*, 2022. DOI: 10.1038/s41567-022-01772-z.

[J10] **D. E. Bernal**, A. Ajagekar, S. M. Harwood, S. T. Stober, D. Trenev, and F. You, "Perspectives of Quantum Computing for Chemical Engineering", *AIChE Journal*, e17651, 2022. DOI: 10.1002/aic.17651.

[J11] **D. E. Bernal**, Z. Peng, J. Kronqvist, and I. E. Grossmann, "Alternative regularizations for Outer-Approximation algorithms for convex MINLP", *Journal of Global Optimization*, pp. 1–36, 2022. DOI: 10.1007/s10898-022-01178-4.

[J12] R. Quintero, **D. E. Bernal**, T. Terlaky, and L. F. Zuluaga, "Characterization of QUBO reformulations for the maximum k-colorable subgraph problem", *Quantum Information Processing*, vol. 21, no. 3, pp. 1–36, 2022. DOI: 10.1007/s11128-022-03421-z.

[J13] Q. Chen, E. S. Johnson, **D. E. Bernal**, R. Valentin, S. Kale, J. Bates, J. D. Siirola, and I. E. Grossmann, "Pyomo. GDP: an ecosystem for logic based modeling and optimization development", *Optimization and Engineering*, pp. 1–36, 2021. DOI: 10.1007/s11081-021-09601-7.

[J14] S. Harwood, C. Gambella, D. Trenev, A. Simonetto, **D. E. Bernal**, and D. Greenberg, "Formulating and Solving Routing Problems on Quantum Computers", *IEEE Transactions on Quantum Engineering*, 2021. DOI: 10.1109/TQE.2021.3049230.

[J15] D. A. Liñán, **D. E. Bernal**, J. M. Gómez, and L. A. Ricardez-Sandoval, "Optimal synthesis and design of catalytic distillation columns: A rate-based modeling approach", *Chemical Engineering Science*, vol. 231, p. 116 294, 2021. DOI: 10.1016/j.ces.2020.116294.

[J16] H. A. Pedrozo, S. R. Reartes, **D. E. Bernal**, A. Vecchietti, M. S. Díaz, and I. E. Grossmann, "Hybrid model generation for superstructure optimization with Generalized Disjunctive Programming", *Computers & Chemical Engineering*, vol. 154, p. 107 473, 2021. DOI: 10.1016/j.compchemeng.2021.107473.

[J17] **D. E. Bernal**, S. Vigerske, F. Trespalacios, and I. E. Grossmann, "Improving the performance of DICOPT in convex MINLP problems using a feasibility pump", *Optimization Methods and Software*, vol. 35, no. 1, pp. 171–190, 2020. DOI: 10.1080/10556788.2019.1641498.

[J18] T. J. Ikonen, H. Mostafaei, Y. Ye, **D. E. Bernal**, I. E. Grossmann, and I. Harjunkoski, "Large-scale selective maintenance optimization using bathtub-shaped failure rates", *Computers & Chemical Engineering*, vol. 139, p. 106 876, 2020. DOI: 10.1016/j.compchemeng.2020.106876.

[J19] J. Kronqvist, **D. E. Bernal**, and I. E. Grossmann, "Using regularization and second order information in outer approximation for convex MINLP", *Mathematical Programming*, vol. 180, no. 1, pp. 285–310, 2020. DOI: 10.1007/s10107-018-1356-3.

[J20] C. Li, **D. E. Bernal**, K. C. Furman, M. A. Duran, and I. E. Grossmann, "Sample average approximation for stochastic nonconvex mixed integer nonlinear programming via outer-approximation", *Optimization and Engineering*, pp. 1–29, 2020. DOI: 10.1007/s11081-020-09563-2.

[J21] D. A. Liñán, **D. E. Bernal**, L. A. Ricardez-Sandoval, and J. M. Gómez, "Optimal design of superstructures for placing units and streams with multiple and ordered available locations. Part I: A new mathematical framework", *Computers & Chemical Engineering*, p. 106 794, 2020. DOI: 10.1016/j.compchemeng.2020.106794.

[J22] D. A. Liñán, **D. E. Bernal**, L. A. Ricardez-Sandoval, and J. M. Gómez, "Optimal design of superstructures for placing units and streams with multiple and ordered available locations. Part II: Rigorous design of catalytic distillation columns", *Computers & Chemical Engineering*, p. 106 845, 2020. DOI: 10.1016/j.compchemeng.2020.106845.

[J23] H. Yang, **D. E. Bernal**, R. E. Franzoi, F. G. Engineer, K. Kwon, S. Lee, and I. E. Grossmann, "Integration of Crude-Oil Scheduling and Refinery Planning by Lagrangean Decomposition", *Computers & Chemical Engineering*, p. 106 812, 2020. DOI: 10.1016/j.compchemeng.2020.106812.

[J24] J. Kronqvist, **D. E. Bernal**, A. Lundell, and I. E. Grossmann, "A review and comparison of solvers for convex MINLP", *Optimization and Engineering*, vol. 20, no. 2, pp. 397–455, 2019. DOI: 10.1007/s11081-018-9411-8.

[J25] J. Kronqvist, **D. E. Bernal**, A. Lundell, and T. Westerlund, "A center-cut algorithm for quickly obtaining feasible solutions and solving convex MINLP problems", *Computers & Chemical Engineering*, vol. 122, pp. 105–113, 2019. DOI: 10.1016/j.compchemeng.2018.06.019.

[J26] C. L. Lara, **D. E. Bernal**, C. Li, and I. E. Grossmann, "Global optimization algorithm for multi-period design and planning of centralized and distributed manufacturing networks", *Computers & Chemical Engineering*, vol. 127, pp. 295–310, 2019. DOI: 10.1016/j.compchemeng.2019.05.022.

[J27] **D. E. Bernal**, C. Carrillo-Diaz, J. M. Gómez, and L. A. Ricardez-Sandoval, "Simultaneous design and control of catalytic distillation columns using comprehensive rigorous dynamic models", *Industrial & Engineering Chemistry Research*, vol. 57, no. 7, pp. 2587–2608, 2018. DOI: 10.1021/acs.iecr.7b04205.

[J28] L. Su, L. Tang, **D. E. Bernal**, and I. E. Grossmann, "Improved quadratic cuts for convex mixed-integer nonlinear programs", *Computers & Chemical Engineering*, vol. 109, pp. 77–95, 2018, ISSN: 0098-1354. DOI: 10.1016/j.compchemeng.2017.10.011.

[J29] L. Leisman, M. P. Haynes, S. Janowiecki, G. Hallenbeck, G. Józsa, R. Giovanelli, E. A. Adams, **D. E. Bernal**, J. M. Cannon, W. F. Janesh, *et al.*, "(Almost) Dark Galaxies in the ALFALFA Survey: Isolated H i-bearing Ultra-diffuse Galaxies", *The Astrophysical Journal*, vol. 842, no. 2, p. 133, 2017. DOI: 10.3847/1538-4357/aa7575.

Conference Proceedings

[P1] R. A. Brown, D. Venturelli, M. Pavone, and **D. E. Bernal**, "Accelerating continuous variable coherent ising machines via momentum", in *International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research*, **(CPAIOR2024)**, Springer, 2024, pp. 109–126. DOI: 10.1007/978-3-031-60597-0_8.

[P2] A. F. Cabeza, A. Orjuela, and **D. E. Bernal**, "A novel cost-efficient tributyl citrate production process", in *Proceedings of the 10th International Conference on Foundations of Computer Aided Process Design (FOCAPD 2024)*, ser. Systems & Controls Transactions, vol. 3, **(FOCAPD2024)**, PSE Press: Hamilton, 2024, pp. 121–128, ISBN: 978-1-7779403-2-4.

[P3] A. F. Cabeza, A. Orjuela, and **D. E. Bernal**, "Analysis of Calcium Citrate Salts as Raw Material for Tributyl Citrate Bio-Plasticizer Production: Kinetic Modeling, Process Simulation, and Optimization", in *Computer Aided Chemical Engineering*, vol. 53, **(PSE2024/ESCAPE34)**, Elsevier, 2024, pp. 955–960. DOI: 10.1016/B978-0-443-28824-1.50160-5.

[P4] Z. Peng, K. Cao, K. C. Furman, C. Li, I. E. Grossmann, and **D. E. Bernal**, "A convexification-based outer-approximation method for convex and nonconvex minlp", in *Proceedings of the 34th European Symposium on Computer Aided Process Engineering*, **(PSE2024/ESCAPE34)**, Elsevier, vol. 53, 2024. DOI: 10.1016/B978-0-443-28824-1.50536-6.

[P5] F. Sorourifar, D. Chamaki, N. M. Tubman, J. Paulson, and **D. E. Bernal**, "Bayesian optimization priors for efficient variational quantum algorithms", in *Computer Aided Chemical Engineering*, vol. 53, **(PSE2024/ESCAPE34)**, Elsevier, 2024, pp. 3379–3384. DOI: 10.1016/B978-0-443-28824-1.50564-0.

[P6] C. Tristán, M. Fallanza, R. Ibáñez, I. E. Grossmann, and **D. E. Bernal**, "Designing reverse electrodialysis process for salinity gradient power generation via disjunctive programming", in *Proceedings of the 10th International Conference on Foundations of Computer Aided Process Design (FOCAPD 2024)*, ser. Systems & Controls Transactions, vol. 3, **(FOCAPD2024)**, PSE Press: Hamilton, 2024, pp. 904–911, ISBN: 978-1-7779403-2-4.

[P7] C. Tristán, M. Fallanza, R. Ibáñez, I. E. Grossmann, and **D. E. Bernal**, "Global optimization via quadratic disjunctive programming for water networks design with energy recovery", in *Computer Aided Chemical Engineering*, vol. 53, **(PSE2024/ESCAPE34)**, Elsevier, 2024, pp. 2161–2166. DOI: 10.1016/B978-0-443-28824-1.50361-6.

[P8] P. M. Xavier, P. Ripper, J. Pulsipher, J. D. Garcia, N. Maculan, and **D. E. Bernal**, "Disjunctive programming meets qubo", in *Computer Aided Chemical Engineering*, vol. 53, **(PSE2024/ESCAPE34)**, Elsevier, 2024, pp. 3433–3438. DOI: 10.1016/B978-0-443-28824-1.50573-1.

[P9] N. P. Sawaya, D. Marti-Dafcik, Y. Ho, D. P. Tabor, **D. E. Bernal**, A. B. Magann, S. Premaratne, P. Dubey, A. Matsuura, N. Bishop, *et al.*, "HamLib: A library of Hamiltonians for benchmarking quantum algorithms and hardware", in *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)*, IEEE, vol. 2, 2023, pp. 389–390.

[P10] **D. E. Bernal**, Y. Liu, M. L. Bynum, C. D. Laird, J. D. Siirola, and I. E. Grossmann, "Advances in generalized disjunctive and mixed-integer nonlinear programming algorithms and software for superstructure optimization", in *Computer Aided Chemical Engineering*, vol. 49, **(PSE2021+)**, Elsevier, 2022, pp. 1285–1290. DOI: 10.1016/B978-0-323-85159-6.50214-1.

[P11] **D. E. Bernal**, D. Ovalle, D. A. Liñán, L. A. Ricardez-Sandoval, J. M. Gómez, and I. E. Grossmann, "Process superstructure optimization through discrete steepest descent optimization: A gdp analysis and applications in process intensification", in *Computer Aided Chemical Engineering*, vol. 49, **(PSE2021+)**, Elsevier, 2022, pp. 1279–1284. DOI: 10.1016/B978-0-323-85159-6.50213-X.

[P12] **D. E. Bernal**, K. E. Booth, R. Dridi, H. Alghassi, S. Tayur, and D. Venturelli, "Integer programming techniques for minor-embedding in quantum annealers", in *International Conference on Integration of Constraint Programming, Artificial Intelligence, and Operations Research*, **(CPAIOR2020)**, Springer, 2020, pp. 112–129. DOI: 10.1007/978-3-030-58942-4_8.

[P13] **D. E. Bernal**, Q. Chen, F. Gong, and I. E. Grossmann, "Mixed-Integer Nonlinear Decomposition Toolbox for Pyomo (MindtPy)", in *13th International Symposium on Process Systems Engineering (PSE 2018)*, ser. Computer Aided Chemical Engineering, vol. 44, **(PSE2018)**, Elsevier, 2018, pp. 895–900. DOI: 10.1016/B978-0-444-64241-7.50144-0.

[P14] L. Su, L. Tang, **D. E. Bernal**, I. E. Grossmann, and B. Wang, "Integrated scheduling of on-line blending and distribution of oil products in refinery operation", in *13th International Symposium on Process Systems Engineering (PSE 2018)*, ser. Computer Aided Chemical Engineering, vol. 44, **(PSE2018)**, Elsevier, 2018, pp. 1213–1218. DOI: 10.1016/B978-0-444-64241-7.50197-X.

Articles Preprints and Under Review

[S1] **D. E. Bernal**, R. Brown, P. Sathe, F. Wudarski, M. Pavone, E. G. Rieffel, and D. Venturelli, "Benchmarking the Operation of Quantum Heuristics and Ising Machines: Scoring Parameter Setting Strategies on Optimization Applications", Submitted for publication. Available here., 2024.

[S2] A. Chatterjee, S. Rappaport, A. Giri, S. Johri, T. Proctor, **D. E. Bernal**, P. Sathe, and T. Lubinski, "A Comprehensive Cross-Model Framework for Benchmarking the Performance of Quantum Hamiltonian Simulations", Submitted for publication. Available here., 2024.

[S3] S. Dutta, P. P. Karanth, P. M. Xavier, I. L. de Freitas, N. Innan, S. B. Yahia, M. Shafique, and **D. E. Bernal**, "Federated Learning with Quantum Computing and Fully Homomorphic Encryption: A Novel Computing Paradigm Shift in Privacy-Preserving ML", Submitted for publication. Available here., 2024.

[S4] E. J. Gustafson, J. Tiihonen, D. Chamaki, F. Sorourifar, J. W. Mullinax, A. C. Li, F. B. Maciejewski, N. P. Sawaya, J. T. Krogel, **D. E. Bernal**, and N. Tubman, "Surrogate optimization of variational quantum circuits", Submitted for publication. Available here., 2024.

[S5] P. Kerger, **D. E. Bernal**, Z. Gonzalez Izquierdo, and E. G. Rieffel, "Classical and Quantum Distributed Algorithms for the Survivable Network Design Problem", Submitted for publication. Available here., 2024.

[S6] F. B. Maciejewski, B. G. Bach, M. Dupont, P. A. Lott, B. Sundar, **D. E. Bernal**, I. Safro, and D. Venturelli, "A Multilevel Approach For Solving Large-Scale QUBO Problems With Noisy Hybrid Quantum Approximate Optimization", Submitted for publication. Available here., 2024.

[S7] Z. Peng, A. Lee, and **D. E. Bernal**, "Addressing Discrete Dynamic Optimization via a Logic-Based Discrete-Steepest Descent Algorithm", Submitted for publication. Available here., 2024.

[S8] W. Chaimanowong, **D. E. Bernal**, and F. Cisternas, "Optimizing Product Influence of Shelf Display", Submitted for publication. Available here., 2023.

[S9] P. Maciel Xavier, P. Ripper, T. Andrade, J. Dias Garcia, N. Maculan, and **D. E. Bernal**, "QUBO.jl: A Julia Ecosystem for Quadratic Unconstrained Binary Optimization", Submitted for publication. Available here., 2023.

[S10] **D. E. Bernal**, S. Tayur, and D. Venturelli, "Quantum Integer Programming (QuIP) 47-779: Lecture Notes", Available here., 2020.

Invited Seminars and Lectures

- Panelist: Artificial Intelligence in Chemical Engineering - IV Symposium of Applied Optimization in Chemical Engineering (SOAIQ), Intituto Tecnologico de Monterrey, Mexico 10/2024
- Invited Seminar: Perspectives of Quantum Computing for Chemical Engineering - Universidad de Guanajuato, Mexico 10/2024
- Seminar: Quantum-Classical Hybrid Methods: Applications in optimization, machine learning, and computational chemistry - Qiskit Fall Fest IBM, Quantum Computing School in Spanish 09/2024
- Invited Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Key Laboratory of Data Analytics and Optimization for Smart Industry, Northeastern University, Shenyang, China 04/2024
- Invited Seminar: Quantum Computing for PSE. Opportunities via Problem Decomposition for Optimization, Machine Learning, and Computational Chemistry - 3rd Process Systems Engineering State of the Art Workshop, Hangzhou, China 04/2024
- Seminar: Perspectives on Quantum Computing for Chemical Engineering - Energy and Process Systems Engineering, ETH, Zurich, Switzerland 03/2024
- Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Technology Innovation Institute, Abu Dhabi, United Arab Emirates 03/2024
- Invited Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Industrial and Systems Engineering Research Seminar, Lehigh University, Bethlehem, PA, USA 02/2024
- Panelist: Navigating the Intersection of Technology and Society - Purdue Engineering Distinguished Lecture Series of Dean Yannis Yortsos, Purdue University, West Lafayette, IN, USA Video 01/2024
- Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Midwest Quantum Collaboratory Seminar, Purdue University, West Lafayette, IN, USA December. 2023
- Invited Lecture: Perspectives on Quantum Computing for Chemical Engineering - Department of Chemical Engineering, Universidad Nacional de Colombia, Bogotá, Colombia 11/2023
- Invited Lecture: Quantum Computing Tutorial - Machine Learning for Engineering, Universidad de los Andes, Bogotá, Colombia 11/2023
- Panelist: Artificial Intelligence and Superior Education - AI and Education Congress, Universidad Central, Bogotá, Colombia 10/2023
- Seminar: Quantum and Quantum-Inspired Methods for Optimization: Modeling, Algorithms, and Perspectives - Qiskit Fall Fest IBM, Quantum Computing School in Spanish Video 10/2023
- Invited Panelist: Quantum Computing - 9th Arab-American Frontiers Symposium, National Academies of Science, Engineering, and Medicine, Doha, Qatar 10/2023
- Invited Seminar: Quantum and Quantum-Inspired Methods for Optimization: Modeling, Algorithms, and Perspectives - 9th Arab-American Frontiers Symposium, National Academies of Science, Engineering, and Medicine, Doha, Qatar 10/2023
- Seminar: Perspectives on Quantum Computing for Chemical Engineering - IChemE Webinar series Video 10/2023
- Invited Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Industrial Engineering Research Seminar, Purdue University, West Lafayette, IN, USA 09/2023

- Panelist: Artificial Intelligence and Superior Education - AI and Education Congress, Fundación Alberto Merani, Bogotá, Colombia 08/2023
- Invited Speaker: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Learning from Both Sides Linear and Nonlinear Mixed-Integer Optimization, Institut Mittag-Leffler, Stockholm, Sweden 07/2023
- Seminar: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - Power Systems Lab, Department of Information Technology and Electrical Engineering, ETH, Zürich, Switzerland 02/2023
- Seminar: Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry - Sargent Centre of Process Systems Engineering, Imperial College London, London, UK 02/2023
- Seminar: Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry - CODES Research Group Meeting, University of West Virginia, Morgantown, VA, USA 02/2023
- Lecture: Discrete nonlinear optimization: Modeling and solutions via novel hardware and decomposition algorithms - 5th Grid Science Winter School - Los Alamos National Laboratory, Santa Fe, NM, USA 01/2023
- Seminar: Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry - Sustainable Process Systems Engineering Lab, Institute of Chemical and Bioengineering, ETH, Zürich, Switzerland 12/2022
- Seminar: Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry - Department of Chemical Engineering, McMaster University, Hamilton, ON, Canada 10/2022
- Seminar: Exploiting and Benchmarking Ising Solvers - Quantum Pittsburgh (QPitt) Meetup, Pittsburgh, PA, USA 10/2022
- Seminar: Introduction to Quantum Computing and Perspectives of Quantum Computing for Chemical Engineering - Quantum Pittsburgh (QPitt) Meetup, Pittsburgh, PA, USA 06/2022
- Plenary Moderator and Panelist: Future of Quantum Computing in Optimization - 2022 CORS/INFORMS International Conference, Vancouver, Canada 06/2022
- Seminar: Quantum Computing and Modern Computational Optimization Approaches to Process Systems Engineering - Laboratoire d'Informatique de Paris Nord, Paris, France 04/2022
- Seminar: Quantum Computing and Modern Computational Optimization Approaches to Process Systems Engineering (in Spanish) - Universidad de los Andes, Bogotá, Colombia 01/2022
- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization and Process Systems Engineering (in Spanish) - Universidad Nacional de Colombia, Bogotá, Colombia 12/2021
- Plenary: Modern Computational Approaches to Nonlinear Discrete Optimization and Process Systems Engineering (in Spanish) - Argentinian Symposium on Industrial Computing and Operations Research, Argentina Video 08/2021
- Quantum Computing for Discrete Nonlinear Optimization. Graver Augmented Multiseed Algorithm - Mixed-Integer Nonlinear Programming Virtual Workshop, Computational Optimization Group, Imperial College, London, UK Video 06/2021
- Invited Lecture for Modeling and Optimization Group, PSR, Rio de Janeiro, Brazil 04/2021
- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization - Quantum Computing and Mathematical Optimization, Real World Optimization meeting, Gesellschaft für Operations Research and German Aerospace Center, Germany 03/2021
- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization and Applications in Process Systems Engineering - Group for Applied Mathematical Modeling and Analytics, Industrial Engineering Department, University at Buffalo, NY, USA 03/2021
- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization (in Spanish) - Chemical Engineering Department, Universidad de Salamanca, Salamanca, Spain 01/2021
- Invited Lecture for Modeling and Optimization Journal Club: Quantum Computing for Optimization - Modeling and Optimization, Amazon, Seattle, WA, USA 01/2021
- Invited Lecture for 17-617 Programming Quantum Computers: Quantum Annealing and Ising Model Computation - Institute for Software Research, Carnegie Mellon University, Pittsburgh, PA, USA 12/2020

- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization and their Application to Process Systems Engineering - Chemical Engineering Future Faculty Series 12/2020
- Seminar: Modern Computational Approaches to Nonlinear Discrete Optimization and their Application to Process Systems Engineering - Discrete Optimization Talks (DOT) Video 12/2020
- Invited Distinguished Speaker: Modern computational approaches to nonlinear discrete optimization - Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, USA 11/2020
- Invited Lecture for ID5840 Quantum Integer Programming – Department of Electrical Engineering, Indian Institute of Technology, Madras, India 10/2020
- Invited Lecture for 06-720 Advanced Process Systems Engineering: Constraint Programming - Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA, USA 02/2020
- Invited Lecture for 47-830 Integer Programming: Valid inequalities for Mixed-Integer Programming - Tepper School of Business, Carnegie Mellon University, Pittsburgh, PA, USA 02/2019
- Seminar: Incorporating Quadratic Approximations in the Outer-Approximation Method for Convex MINLP - Universidad Nacional del Litoral, Santa Fé, Argentina 08/2018
- Incorporating Quadratic Approximations in the Outer-Approximation Method for Convex MINLP - Designing and Implementing Algorithms for Mixed-Integer Nonlinear Optimization, Dagstuhl Seminar 18081, Dagstuhl, Germany 02/2018

Invited Conference Presentations

1. Bhatia, A.S., **Bernal, D.E.**. "Federated Hierarchical Tensor Networks: a Collaborative Quantum AI-Driven Framework for Healthcare", *2024 Institute For Operations Research and Management Science (INFORMS) Optimization Society (OS) Meeting.*
2. Lubinski, T., Coffrin, C., McGeoch, C., Sathe, P., Apanavicius, J., **Bernal, D.E.**. "Optimization Applications as Quantum Performance Benchmarks", *2024 INFORMS OS (IOS) Meeting.*
3. **Bernal, D.E.**, Brown, R., Sathe, P., Wudarski, P., Pavone, M., Rieffel, E., Venturelli, D.. "Benchmarking the Operation of Quantum Heuristics and Ising Machines: Scoring Parameter Setting Strategies on Optimization Applications", *2024 IOS Meeting.*
4. **Bernal, D.E.** "Using Quantum and Physics-Inspired Methods for Constrained Optimization: Reformulations, Decomposition Algorithms, Software and Benchmarking", *2023 Institute for Operations Research and Management Sciences (INFORMS) Meeting.*
5. Brown, R., **Bernal, D.E.**, Venturelli, D., Pavone, M. "Accelerating Coherent Continuous Variable Machines Using Momentum", *2023 INFORMS Meeting.*
6. Sorourifar, F., Chamaki, D., Tubman, N, Paulson, J., **Bernal, D.E.** "Specialized Gaussian Process Modifications for Shot-Efficient Quantum-Classical Optimization", *2023 INFORMS Meeting.*
7. Peng, Z., Grossmann, I.E., **Bernal, D.E.** "Mixed-Integer Nonlinear Decomposition Toolbox in Pyomo", *2023 INFORMS Meeting.*
8. **Bernal, D.E.**, Brown, R.A., Venturelli, D., Pavone, M. "Hybrid Classical-Quantum Algorithms for Mixed-Integer Optimization", *2023 Society of Industrial and Applied Mathematics Optimization Meeting (SIAM OP23).*
9. **Bernal, D.E.**, Venturelli, D., Wudarski, F.A., Rieffel, E.G. "Benchmarking the Operation of Quantum Heuristics and Ising Machines: Scoring Parameter Setting Strategies on Real World Optimization Applications", *2022 INFORMS Meeting.*
10. Brown, R.A., **Bernal, D.E.**, Venturelli, D., Pavone, M. "Copositive Optimization via Ising Solvers", *2022 INFORMS Meeting.*
11. Rieffel, E., Kerger, P., **Bernal, D.E.**. "Quantum, quantum-classical hybrid, and distributed quantum algorithms for problems in operations research", *Workshop on Quantum Computing and Operations Research 2022.*
12. **Bernal, D.E.**. Plenary Moderator and Panelist "Future of Quantum Computing in Optimization", *2022 CORS/INFORMS International Conference.*

13. **Bernal, D.E.**, Grossmann, I.E. "Easily Solvable Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming using Cones", *2021 INFORMS Meeting.*
14. Quintero, R.A., **Bernal, D.E.**, Terlaki, T., Zuluaga, L., "Characterization of QUBO reformulations for the maximum k-colorable subgraph problem", *2021 INFORMS Meeting.*
15. **Bernal, D.E.**, Peng, Z., Kronqvist, J., Grossmann, I.E. "Regularization in Decomposition Methods for Global Optimization of Mixed-Integer Nonlinear Programming", *31st European Conference on Operational Research (EURO) 2021.*
16. Li, C., Grossmann, I.E., **Bernal, D.E.**, Furman, K., "Sample Average Approximation for Stochastic Nonconvex Mixed Integer Nonlinear Programming via Outer Approximation", *31st EURO 2021.*
17. Quintero, R.A., **Bernal, D.E.**, Terlaki, T., Zuluaga, L., "Characterization of QUBO reformulations for the maximum k-colorable subgraph problem", *31st EURO 2021.*
18. **Bernal, D.E.**, Kronqvist, J., Lundell, A., Grossmann, I.E. "A Review And Comparison Of Solvers For Convex MINLP", *2020 INFORMS Meeting.*
19. Li, C., **Bernal, D.E.**, Grossmann, I.E., Furman, K., "Sample Average Approximation for Stochastic Nonconvex Mixed Integer Nonlinear Programming via Outer Approximation", *2020 INFORMS Meeting.*
20. **Bernal, D.E.**, Valentin, R., Chen, Q., Grossmann, I.E. "Mixed-integer Nonlinear Decomposition Toolbox for Pyomo MindtPy", *2019 INFORMS Meeting.*
21. Chen, Q., Valentin, R., Kale, S., Bates, J., **Bernal, D.E.**, Bynum, M.L., Siirola, J., Grossmann, I.E. "Advances in Pyomo.GDP: an Ecosystem For Nonlinear Disjunctive Programming Modeling and Optimization Development", *2019 INFORMS Meeting.*
22. **Bernal, D.E.**, Gong, F., Chen, Q., Grossmann, I.E. "Mixed-integer Nonlinear Decomposition Toolbox for Pyomo", *2018 INFORMS Meeting.*
23. **Bernal, D.E.**, Kronqvist, J., Lundell, A., Westerlund, T., Grossmann, I.E. "A Center Cut Algorithm for Quickly Obtaining Feasible Solutions and Solving Convex Mixed Integer Nonlinear Programs", *2018 INFORMS Meeting.*
24. Yang, H., **Bernal, D.E.**, Grossmann, I.E. "Integration of Crude-Oil Scheduling and Refinery Planning By Lagrangean Decomposition Approach", *2018 INFORMS Meeting.*

Contributed Conference Presentations

1. **Bernal, D.E.**, Peng, Z., Furman, K., Li, C., Grossmann, I.E., "A Convexification-Based Outer-Approximation Method for Convex and Nonconvex MINLP", *25th International Symposium of Mathematical Programming (ISMP2024).*
2. **Bernal, D.E.**, Peng, Z., Maciel Xavier, P."Hybrid Quantum Branch-and-Bound Method for Quadratic Unconstrained Binary Optimization", *ISMP2024.*
3. Maciel Xavier, P., Ripper, P., Dias Garcia, J., Maculan, N.,**Bernal, D.E.**, "QUBO.jl: A tale of implementation and benchmarking of a Quantum Optimization Ecosystem in Julia", *ISMP2024.*
4. **Bernal, D.E.**, Peng, Z., Maciel Xavier, P."Hybrid Quantum Branch-and-Bound Method for Quadratic Unconstrained Binary Optimization", *Julia Mathematical Programming developers workshop 2024 (JuMP-dev 2024)*, Video.
5. Maciel Xavier, P., Ripper, P., Dias Garcia, J., Maculan, N.,**Bernal, D.E.**, "QUBO.jl: A tale of implementation and benchmarking of a Quantum Optimization Ecosystem in Julia", *JuMP-dev 2024*, Video.
6. Lee, A., Ovalle, D. Liñán, D.A., Ricardez-Sandoval, L., Gómez, J.M., Grossmann, I.E., **Bernal, D.E.**. "Logic-Based Discrete-Steepest Descent: A Solution Method for Process Synthesis Generalized Disjunctive Programs", *2024 American Institute of Chemical Engineers (AIChE) Midwest Regional Conference.*
7. Tristán, C., Fallanza, M., Ibañez, R., **Bernal, D.E.**. "Optimizing Reverse Electrodialysis Process for Renewable Electricity Generation from Salinity Gradient", *2024 AIChE Midwest Regional Conference.*
8. **Bernal, D.E.**, Kerger, P., Rieffel E. "Classical and Quantum Distributed Algorithms for the Survivable Network Design Problem", *2024 American Physics Society (APS) March Meeting.*
9. Gustafson, E., Tiihosen, J., Chamaki, D., Mullinax, W., **Bernal, D.E.**, Swaya, N., Maciejewski, F., Kim, J., Tubman, N., Krogel, J. "Surrogate Optimization for Quantum Circuits", *2024 APS March Meeting.*

10. Chamaki, D., Sorourifar, F., Velury, S., Hargus, C., Klymko, K., Hamilton, K., Hadfield, S., Mullinax, W., Paulson, J., **Bernal, D.E.**, Rotskoff, G., Tubman, N. "A look at the truths and misconceptions of the variational quantum eigensolver and the implications of overparameterization", *2024 APS March Meeting*.
11. Cabeza, A.F., Orjuela, A., **Bernal, D.E.** "Tributyl Citrate production from Calcium Citrate Salt: Reaction Kinetics and Process Simulation", *2023 American Institute of Chemical Engineering (AIChE) Meeting*.
12. Peng, Z., Grossmann, I.E., **Bernal, D.E.** "Mixed-Integer Nonlinear Decomposition Toolbox in Pyomo", *2023 AIChE Meeting*.
13. **Bernal, D.E.**, Kerger, P., Rieffel, E.G., "Quantum Distributed Algorithms for Approximate Steiner Trees and Directed Minimum Spanning Trees", *2023 APS March Meeting*.
14. Sathe, P., Lubinski, T., Coffrin, C., Apanavicius, J., McGeoch, C., **Bernal, D.E.** "Characteristics of Optimization Applications as Quantum Performance Benchmarks", *2023 APS March Meeting*.
15. Quintero, R.A., **Bernal, D.E.**, Terlaki, T., Zuluaga, L., "Characterization of QUBO reformulations for the maximum k-colorable subgraph problem", *XXI Latin-Iberoamerican Conference on Operations Research (CLAIO) 2022*.
16. **Bernal, D.E.** "Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry", *2022 AIChE Meeting*.
17. **Bernal, D.E.**, Brown, R.A., Venturelli, D., Pavone, M. "Mixed-Binary Quadratic Programming via Convex Copositive Optimization and Ising Solvers", *7th International Conference on Continuous Optimization (ICCOPT) 2022*.
18. Brown, R.A., **Bernal, D.E.**, Sahasrabudhe, A., Loot, A., Venturelli, D., Pavone, M. "Copositive optimization via Ising solvers", *24th International Conference on the Integration of Constraint Programming, Artificial Intelligence, and Operations Research (CPAIOR) 2022*, Video.
19. **Bernal, D.E.** "Perspectives on Quantum Computing for Chemical Engineering: A joint view from Academia and Industry", *2022 Quantum Computing Applications in Chemical and Biochemical Engineering Workshop*.
    - Prize for best talk at the workshop
20. **Bernal, D.E.**, Venturelli, D., Wudarski, F.A., Rieffel, E.G. "Benchmarking the Operation of Quantum Heuristics and Ising Machines: Scoring Parameter Setting Strategies on Real World Optimization Applications", *2022 APS March Meeting*.
21. **Bernal, D.E.**, Peng, Z., Kronqvist, J., Grossmann, I.E. "Alternative Regularization Schemes in Outer-Approximation Algorithms for Convex MINLP", *2021 AIChE Meeting*.
22. **Bernal, D.E.**, Ovalle, D., Liñán, D., Gómez, J.M., Ricardez-Sandoval, L., Grossmann, I.E. "Discrete-Steepest Descent: A Solution Method for Process Synthesis Generalized Disjunctive Programs", *2021 AIChE Meeting*.
23. Pedrozo, A., Rodriguez, S.B., **Bernal, D.E.**, Vechietti, A., Diaz, M.S., Grossmann, I.E. "Optimal Synthesis and Heat Integration Using Generalized Disjunctive Programming with Hybrid Models", *2021 AIChE Meeting*.
24. **Bernal, D.E.**, Peng, Z., Kronqvist, J., Grossmann, I.E. "Regularization in Decomposition Methods for Global Optimization of Mixed-Integer Nonlinear Programming", *2021 Society for Industrial and Applied Mathematics (SIAM) Conference on Optimization*.
25. **Bernal, D.E.** "Modern Computational Approaches to Nonlinear Discrete Optimization and Their Application to Process Systems Engineering", *2020 AIChE Meeting*.
    - Meet the Faculty & Post-Doc Candidates Poster Session
26. **Bernal, D.E.**, Grossmann, I.E. "Use of Quantum Computing to Solve Optimization Problems in Process Systems Engineering", *2020 AIChE Meeting*.
    - Computing and Systems Technology Division Directors' Student Award Finalist
27. Li, C., **Bernal, D.E.**, Grossmann, I.E., Furman, K., "Sample Average Approximation for Stochastic Nonconvex Mixed Integer Nonlinear Programming via Outer Approximation", *2020 AIChE Meeting*.
28. Chen, Q., **Bernal, D.E.**, Johnson, E., Valentin, R., Kale, S., Bates, J., Siirola, J.D., Grossmann, I.E. "Pyomo.GDP: An Ecosystem for Logic-Based Modeling and Optimization Development", *2020 AIChE Meeting*.
29. Chen, Q., Liu Y., Seastream G., **Bernal, D.E.**, Siirola, J.D., Grossmann, I.E. "Pyosyn Graph: New Representation and Systematic Generation of Process Superstructures", *2020 AIChE Meeting*.

30. **Bernal, D.E.**, Booth, K.E.C., Dridi, R., Alghassi, H., Tayur, S., Venturelli, D. "Integer Programming techniques for minor-embedding in quantum annealers", *Constraint Programming, Artificial Intelligence, Operations Research CPAIOR 2020.*
31. **Bernal, D.E.**, Grossmann, I.E. "Easily Solvable Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming using Cones", *2019 AIChE Meeting.*
32. Chen, Q., Kale, S., Bates, J., Romeo, V., **Bernal, D.E.**, Bynum, M., Siirola, J.D., Grossmann, I.E. "Pyosyn: A Collaborative Ecosystem for Process Design Advancement", *2019 AIChE Meeting.*
33. **Bernal, D.E.**, Su, L., Tang, L., Grossmann, I.E. "Quadratic Cut Decomposition Method for Convex Mixed-Integer Nonlinear Programs", *2018 AIChE Meeting.*
34. Yang, H., **Bernal, D.E.**, Grossmann, I.E. "Integration of Crude-Oil Scheduling and Refinery Planning By Lagrangean Decomposition Approach", *2018 AIChE Meeting.* • Best submission in the Refining and Petrochemical Plant Modeling and Operations Improvement Session
35. Su, L., Tang, L., **Bernal, D.E.**, Grossmann, I.E., Wang, B. "Integrated Scheduling of On-Line Blending and Distribution of Oil Products in Refinery Operation", *13th International Symposium on Process Systems Engineering PSE 2018*
36. Kronqvist, J., **Bernal, D.E.**, Grossmann, I.E. "A Level-Based Quadratic Outer-Approximation Algorithm for convex MINLP", *2017 AIChE Meeting.*
37. **Bernal, D.E.**, Gomez, J.M. "Optimal design and control of a catalytic distillation column. Case study: Ethyl tert-butyl ether (ETBE) synthesis column", *2016 AIChE Meeting.*
38. **Bernal, D.E.**, Vigerske, S., Trespalacios, F., Grossmann, I.E. "Feasibility pump for solving convex MINLP problems with DICOPT", *2016 AIChE Meeting.*

Theses

[T1] **D. E. Bernal**, "Modern Computational Approaches to Nonlinear Discrete Optimization and Applications in Process Systems Engineering.", Ph.D. Thesis available here, Ph.D. dissertation, Carnegie Mellon University, 2021.

[T2] **D. E. Bernal**, *Optimal design and control of a catalytic distillation column. Case study: Ethyl tert-butyl ether (ETBE) synthesis column.* M.Sc. Thesis available here, 2017.

[T3] **D. E. Bernal**, *Bounding the tangential velocities of Andromeda's satellite galaxies using nonlinear programming.* B.S. Thesis available (in Spanish) here, 2016.

[T4] **D. E. Bernal**, *Comparative study of the simulation methods of the extractive distillation system for the dehydration of ethanol using glycerol as a solvent.* B.S. Thesis available (in Spanish) here, 2014.

Fellowships and Scholarships

• Efficient mapping quadratic integer programming problems into qudits-based architectures ($50k) 2024
Quantum Collaborative Summit Seed funds

• NSF Supplement Award 2234175 Enabling Quantum Computing Platform access ($50k) 2023
NSF Proposal "Digital design of a network of distributed modular and agile manufacturing systems with optimal supply chain for personalized medical treatments." 2132142

• NSF Supplement Award 2038247 Enabling Quantum Computing Platform access ($50k) 2020
NSF Proposal "GOALI: Optimal Design and Operation of Reliable Process Systems." 1705372

• Travel Award to attend CRM/DIMACS Workshop on Mixed-Integer Nonlinear Programming 2019
Centre de recherches mathématiques and Center for Discrete Mathematics and Theoretical Computer Science

• Feynman Quantum Academy - Internship Program 2019
University Space Research Association (USRA), NASA Quantum and Artificial Intelligence Laboratory

• NSF Travel Award 1838086 2018
NSF Proposal "GOALI: Optimal Design and Operation of Reliable Process Systems." 1705372

• Travel Award to attend COIN fORgery workshop 2019
Institute for Mathematics and its Applications and Computational Infrastructure for Operations Research

• Travel Award to attend Dagstuhl seminar on Mixed-Integer Nonlinear Optimization 2018
NSF Support Grant for Junior Researchers CNS-1257011 and Schloss Dagstuhl Leibniz'Zentrum für Informatik

• Fellowship for Ph.D. in Chemical Engineering 2017
Center of Advanced Decision-making (CAPD), Chemical Engineering Department, Carnegie Mellon University

• Undergraduate Research Fellow in Astrophysics SURF Cornell-UniAndes 2016
Cornell University and Universidad de los Andes

• Fellowship for Master of Science Degree in Chemical Engineering 2014
Chemical Engineering Department, Universidad de los Andes

• Young Engineers Scholarship for International Exchange at Otto-von-Guericke Universität 2012
German Academic Exchange Service (DAAD), Colombian Science National System (COLCIENCIAS), and Universidad de los Andes

• Alberto Magno Scholarship to Academic Excellence 2009
Universidad de los Andes

Memberships and Service

Purdue University West Lafayette, IN, USA

Member of the Center of Quantum Technologies (CQT) 2023-Current

Member of the Center of Innovative and Strategic Transformation of Alkane Resources (CISTAR) 2023-Current

Member of the Purdue Quantum Science and Engineering Institute (PQSEI) 2023-Current

Reviewer of the application of the inaugural 38 by 38 award of the College of Engineering Fall 2024

Member of the Ph.D. recruitment committee at the Davidson School of Chemical Engineering Fall 2023-Current

Faculty co-advisor of the American Institute of Chemical Engineers (AIChE) student chapter Fall 2023-Current

Faculty advisor of the Colombian Student Association Spring 2024-Current

Marshall for the Davidson School of Chemical Engineering graduation Spring 2024

Editorial Activities

- Topic Editor - Frontiers in Computer Science, Experience with Quantum Annealing Computation 2022-2023
- Associate Editor - Frontiers in Chemical Engineering, Computational Methods in Chemical Engineering 2023

Peer Reviewer

- Computers & Chemical Engineering 2020–2024
- Nature Physics 2022–2024
- Industrial & Engineering Chemistry Research 2024
- IEEE Conference in Design and Control 2024
- IEEE Quantum Week - Quantum Machine Learning track 2024
- Digital Chemical Engineering 2022–2023
- Optimization Letters 2021–2022
- ACM Transactions in Quantum Computing 2023
- Quantum Information Processing 2022
- Operational Research 2022
- Frontiers of Sustainability 2022
- IEEE Conference on Decision and Control 2022
- Optimization & Engineering 2019–2021

- Journal of Optimization Theory and Applications 2021
- Quantum Machine Intelligence 2021
- Current Opinion in Chemical Engineering 2021
- Mathematical Programming 2020
- Journal of Global Optimization 2019–2021
- Chemical Engineering Journal 2019
- American Control Conference 2020

Professional Societies Activites

American Institute of Chemical Engineers (AIChE) Member since 2014

- Programming Coordinator at Annual meeting on Applied Mathematics and Numerical Analysis 10D session 2027
- Session co-chair at Annual meeting on advances in process design 10A session 2024
- Organizer for the Workshop of Quantum Computing and Artificial Intelligence for Chemical and Biochemical Engineering Applications - AIChE and DTU 2024
- Session chair at AIChE Midwest Regional Meeting on Machine Learning and Optimizations 2024
- Scientific committee member for the Workshop of Quantum Computing for Chemical and Biochemical Engineering Applications - AIChE and DTU 2023
- Session chair at Workshop of Quantum Computing for Chemical and Biochemical Engineering Applications session on Emerging QC Applications for Engineers 2023
- Jury for the best poster in the Chemical Engineering division for the forum for Latin American chemistry community conference LatinXChemE 2021

Institute for Operations Research and Management Science (INFORMS) Member since 2017

- Program Committee member for Computational Optimization on INFORMS Optimization Society Meeting - Rice University 2024
- Session chair at INFORMS Annual Meeting session on Hybrid Quantum-Classical methods for Optimization and Sampling 2022
- Session chair at INFORMS Annual Meeting session on Integer Programming 2021
- Session chair at INFORMS Annual Meeting session on Pyomo 2019

Society for Industrial and Applied Mathematics (SIAM) Member since 2020

- Organizer of mini-symposium for Quantum Computing in Optimization - SIAM OP meeting 2023

American Physics Society (APS) Member since 2021

- Session chair at APS March Meeting session on Quantum Network Algorithms and Analysis 2023
- Sorting of talks for the Division of Quantum Information at the American Physics Society (APS) March Meeting 2022

Computer Aids for Chemical Engineering Member since 2024

- Session Chair for Education in Process Design session in the Foundations of Computer Aided Process Design (FOCAPD) Meeting 2024

Julia for Mathematical Programming Member of developer team since 2024

- Program committee member for the annual developer meeting https://jump.dev/meetings/jumpdev2024/ 2024
- Session Chair for the annual developer meeting https://jump.dev/meetings/jumpdev2024/ 2024

Carnegie Mellon University Pittsburgh, PA, USA

Member of the Pittsburgh Quantum Institute (PQI) 2019-Current

Chemical Engineering LatinX and Hispanics Graduate Student Recruiting Session Organizer 2021

SHPE Annual Meeting CMU College of Engineering Graduate Student Recruiting Volunteer 2020

Liaison of the CMU Quantum Computing group for the Pittsburgh Quantum Institute (PQI) 2017–2021

Conference chair and organizer of YinzOR Student Conference 2017

Other

Panelist for Workshop on Quantum Computing and Operations Research - Fields Institute in Toronto 2022

Jury for the best undergraduate graduation project at Universidad de los Andes Chemical Engineering 2021

Moderator on the discussion about Decomposition techniques at MINLP Virtual Workshop 2021

Software Products

- **MindtPy** (Developer): Open-source decomposition toolkit for Mixed-Integer Nonlinear Programming
- **Stochastic-Benchmark** (Developer): Open-source benchmarking tool for stochastic optimization solvers
- **toQUBO.jl** (Originator): Open-source library for reformulation of Mathematical Programs into Quadratic Unconstrained Binary Optimization in Julia
- **QUBOTools.jl** (Originator): Open-source Tools for Quadratic Unconstrained Binary Optimization models analysis in Julia
- **QUBODrivers.jl** (Originator): Interface for classical and quantum annealing solvers in Julia
- **GDPLib** (Contributor): Open-source library of Generalized Disjunctive Programming models in Pyomo
- **GDPOpt** (Contributor): Open-source solver for Generalized Disjunctive Programming in Pyomo
- **DICOPT** (Contributor): Commercial solver for Mixed-Integer Nonlinear Programming in GAMS

Complementary Courses Taken

Carnegie Mellon University Pittsburgh, PA, USA

10-716 Advanced Machine Learning, Theory and Methods Spring 2019

10-703 Deep Reinforcement Learning and Control Fall 2019

CAPD Conceptual Design and Optimization Modeling Summer 2015

Universidad de los Andes Bogotá, Colombia

IIND-4101 Advanced Optimization 2014

Universidad Nacional de Colombia Bogotá, Colombia

Advanced Separation Processes 2014

Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg, Germany

5.24 Innovative Concepts in Integrated Reactors 2012

Goethe-Institut Göttingen, Germany

Intensive technical German Course 2012

Skills

- **Programming Languages:** Python, C, FORTRAN, C++, Julia
- **Experience with algebraic modeling language for optimization:** GAMS, Pyomo, AIMMS, JuMP.
- **Software Proficiency:** MATLAB, Aspen Plus, Aspen HYSYS, UniSim Design.

Languages

Level A1/A2 Basic User – B1/B2 Independent User – C1/C2 Proficient User
Common European Framework of Reference for Languages

	Comprehension		Speaking		Written Expression
	Listening	Reading	Oral Interaction	Oral Expression	
Spanish	Native Speaker				
English	C2	C2	C1	C1	C1
	TOEFL 115/120				
German	C1	C1	C1	B2	B2
	Test DaF 4.5/5				
French	A2	A2	A2	A2	A1
	Test Delf A2 74.5/100				