David E. Bernal Neira

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October 12, 2020

RESEARCH INTERESTS

- Theory and applications of machine learning, artificial intelligence, and decision optimization.

- Mixed-integer Nonlinear Programming and Generalized Disjunctive Programming Algorithms and Software.

- Quantum Algorithms for Combinatorial Optimization.

- Special interest in applications in Chemical Engineering and Process Systems Engineering such as Optimal Process Synthesis, Design, Control and Process Intensification.

EDUCATION

Carnegie Mellon University   Pittsburgh, PA, USA
Ph.D. in Chemical Engineering, Advisor: Prof. Ignacio E. Grossmann, GPA: 3.90/4.00   2017–2021

Universidad de los Andes   Bogotá, Colombia
M.S. in Chemical Engineering, GPA: 4.73/5.00   2014–2016

  – Thesis: "Optimal design and control of a catalytic distillation column. Case study: Ethyl tert-butyl ether (ETBE) synthesis column."

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

  – Thesis (in Spanish): "Comparative study of the simulation methods of the extractive distillation system for the dehydration of ethanol using glycerol as a solvent."

B.S. in Physics, GPA: 4.62/5.00   2011–2018

  – Thesis (in Spanish): "Bounding the tangential velocities of Andromeda's satellite galaxies using nonlinear programming."

Otto-von-Guericke Universität   Magdeburg, Germany
International Exchange in Process Engineering   2012–2013

Friedrich Magnus Gesamtschule   Laubach, Germany
Gymnasialabschluss. US equivalent: High School Diploma   2010

Gimnasio Británico   Chía, Colombia
Bilingual High School Diploma. US equivalent: High School Diploma   2009

EXPERIENCE

Carnegie Mellon University – Department of Chemical Engineering   Pittsburgh, PA, USA
Fourth-year PhD Candidate   2017-2021

  – Improvement of algorithms for Mixed-Integer Nonlinear Programming and Generalized Disjunctive Programming.

  – Study of short-term Quantum Computing techniques for combinatorial optimization

  – Maintenance of commercial MINLP solver DICOPT and open-source MINLP solver MindtPy.

Visiting Research Scholar   Summer 2015

  – Evaluation of MINLP heuristic algorithms as improvements for the commercial solver DICOPT.

– Implementation of the improvements as part of the latest version of DICOPT in the software GAMS.

ExxonMobil Engineering and Research Company Clinton, NJ, USA
Ph.D. Intern at Corporate Strategic Research Summer 2020

– Evaluation of quantum computing for solving optimization problems relevant to logistics in oil & gas.
– Comparison of different formulations of Maritime and Vehicle Routing problems for quantum algorithms such as VQE and QAOA, via IBM Qiskit, and Quantum Annealing, via D-Wave Ocean-Tools.

NASA Ames Research Center Mountain view, CA, USA
Ph.D. Intern at the Quantum and Artificial Intelligence Laboratory Summer 2019

– Implementation of Computational Algebraic Geometry compiler for Quantum Annealing problem embedding
– Proposal of Mixed-integer programming formulation of rigorous embedding methods

ExxonMobil Engineering and Research Company Clinton, NJ, USA
Ph.D. Intern at the Process Technology Department Summer 2018

– Development of an optimal operation plan for a combined heat and power plant with carbon capture technologies model.
– Implementation and deployment of model in the software AIMMS.

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

– Researcher by the Process and Products Design Group and the Processes Optimization Group.

Do Analytics LLC. (Industrial optimization model developers) Pittsburgh, PA, USA
Mathematical Programming Analyst Summer 2015

– Exhibitor during the International Symposium of Mathematical Programming (ISMP2015).
– Presenter of the software OPTEX in two sessions of the ISMP2015.

Neyber SAS (Supplier of natural products for the cosmetic and food industry) Bogotá, Colombia
Junior Researcher 2013-2015

– Participant of the design and construction of a vapor extractor and hydro-distiller for essential oils production.
– Developer of new products based on extracts of Colombian endemic plants for the cosmetic industry.
– Exhibitor of these products in fairs in Barcelona (2015), Hamburg (2014), Paris and Frankfurt (2013).

Bayer Technology Services Leverkusen, Germany
Undergraduate Intern Summer 2013

– Modeling of the global effects of dynamic flooding in distillation columns in UniSim Design and automation of this model implementation.
– Modeling of the thermodynamic and electrolytic effects in Hydrochloric Acid absorption in water and implementation of these models into simulation of acid absorption columns.

TEACHING

Carnegie Mellon University Pittsburgh, PA, USA
Course Instructor (one of three) 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 Synthesis Design undergraduate course.	Fall 2017, Fall 2018
– 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

- IQUI-3040 Chemical Process Optimization. 2015-2016
- IQUI-2021 Phase and Chemical Equilibrium. 2014

Undergraduate Teaching Assistant and Grader 2010–2014

- MATE-1203 Differential Calculus and MATE-2301 Differential Equations in the Mathematics Department.
- FISI-1518 Physics 1, FISI-1528 Physics 2, and FISI-2540 Thermodynamics in the Physics Department.
- IQUI-3001 Separation Processes and IQUI-3040 Chemical Process Optimization in the Chemical Engineering Department.

Teaching-related Training

Future Faculty Program - Eberly Center, Carnegie Mellon University 2019–2020

INFORMS Teaching Effectiveness Colloquium 2020

Invited Seminars and Lectures

Upcoming

- Modern Computational Approaches to Nonlinear Discrete Optimization and their Application to Process Systems Engineering - Chemical Engineering Future Faculty Series Dec. 2020
- Quantum Annealing and Ising Model Computation (lecture for 17-617 Programming Quantum Computers) - Institute for Software Research, Carnegie Mellon University, Pittsburgh, PA, USA Nov. 2020
- Modern computational approaches to nonlinear discrete optimization - Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, USA Nov. 2020

  Previous

- Quantum Integer Programming – Department of Electrical Engineering, Indian Institute of Technology, Madras, India Oct. 2020
- Contraint Programming (lecture for 06-720 Advanced Process Systems Engineering) - Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA, USA Feb. 2020
- Mixed-Integer and Disjunctive Optimization Theory, Software, and Algorithms - Institute of Industrial & Systems Engineering, Northeastern University, Shenyang, China April 2019
- Valid inequalities for Mixed-Integer Programming (lecture for 47-830 Integer Programming) - Tepper School of Business, Carnegie Mellon university, Pittsburgh, PA, USA Feb. 2019
- Incorporating Quadratic Approximations in the Outer-Approximation Method for Convex MINLP - Universidad Nacional del Litoral, Santa Fé, Argentina Aug. 2018
- Mathematical Programming in Python: Pyomo Workshop - Instituto de Desarrollo y Diseño INGAR CONICET-Universidad Tecnológica Nacional, Santa Fé, Argentina Aug. 2018

Journal Publications

[J1] **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: doi:10.1080/10556788.2019.1641498.

[J2] 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: https://doi.org/10.1016/j.compchemeng.2020.106876.

[J3]   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: doi.org/10.1007/s10107-018-1356-3.

[J4]   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: doi.org/10.1007/s11081-020-09563-2.

[J5]   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: https://doi.org/10.1016/j.compchemeng.2020.106794.

[J6]   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: https://doi.org/10.1016/j.compchemeng.2020.106845.

[J7]   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: https://doi.org/10.1016/j.compchemeng.2020.106812.

[J8]   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: doi:10.1007/s11081-018-9411-8.

[J9]   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: https://doi.org/10.1016/j.compchemeng.2018.06.019.

[J10]   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: https://doi.org/10.1016/j.compchemeng.2019.05.022.

[J11]   **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: doi.org/10.1021/acs.iecr.7b04205.

[J12]   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: doi.org/10.1016/j.compchemeng.2017.10.011.

[J13]   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: doi.org/10.3847/1538-4357/aa7575.

Conference Proceedings

[P1]   **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: doi.org/10.1007/978-3-030-58942-4_8.

[P2] **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: doi.org/10.1016/B978-0-444-64241-7.50144-0.

[P3] 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: doi.org/10.1016/B978-0-444-64241-7.50197-X.

Conference Presentations

Upcoming

1. **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

2. **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

3. 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*.

4. **Bernal D.E.**, Kronqvist, J., Lundell, A., Grossmann, I.E. "A Review And Comparison Of Solvers For Convex MINLP", *2020 INFORMS Meeting*.

   Previous

5. **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*.

6. **Bernal D.E.**, Grossmann, I.E. "Easily Solvable Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming using Cones", *2019 AIChE Meeting*.

7. **Bernal D.E.**, Valentin, R., Chen, Q., Grossmann I.E. "Mixed-integer Nonlinear Decomposition Toolbox for Pyomo MindtPy", *2019 INFORMS Meeting*.

8. **Bernal D.E.**, Su, L., Tang, L., Grossmann, I.E. "Quadratic Cut Decomposition Method for Convex Mixed-Integer Nonlinear Programs", *2018 AIChE Meeting*.

9. Yang, H., **Bernal D.E.**, Grossmann, I.E. "Integration of Crude-Oil Scheduling and Refinery Planning By Lagrangean Decomposition Approach", *2018 AIChE Meeting*.

   - Best abstract in the Refining and Petrochemical Plant Modeling and Operations Improvement Session

10. **Bernal D.E.**, Gong, F., Chen, Q., Grossmann, I.E. "Mixed-integer Nonlinear Decomposition Toolbox for Pyomo", *2018 INFORMS Meeting*.

11. **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*.

12. 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*

13. Kronqvist, J., **Bernal D.E.**, Grossmann I.E. "A Level-Based Quadratic Outer-Approximation Algorithm for convex MINLP", *2017 AIChE Meeting*.

14. **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.*

15. **Bernal D.E.**, Vigerske, S., Trespalacios, F., Grossmann, I.E. "Feasibility pump for solving convex MINLP problems with DICOPT", *2016 AIChE Meeting.*

Articles in Progress or Under Review

[S1] **D. E. Bernal**, H. Alghassi, R. Dridi, S. Tayur, and I. E. Grossmann, "Evaluating the Quantum inspired Graver Based Algorithm for Integer Nonlinear Programs", In preparation.

[S2] **D. E. Bernal** and I. E. Grossmann, "Easily Solvable Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming using Cones", In preparation.

[S3] **D. E. Bernal**, Z. Peng, and I. E. Grossmann, "Using First-order Regularization in Outer Approximation for Convex MINLP", In preparation.

[S4] **D. E. Bernal**, Z. Peng, C. Li, K. Furman, and I. E. Grossmann, "Implementing Global Outer-Approximation for nonconvex MINLP", In preparation.

[S5] 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", In preparation. Available here.

[S6] R. Quintero, **D. E. Bernal**, T. Terklaky, and L. F. Zuluaga, "Characterization of QUBO Reformulations for the Maximum k-Colorable Subgraph Problem", In preparation. Available here.

[S7] S. Harwood, C. Gambella, D. Trenev, A. Simonetto, and **D. E. Bernal**, "Formulating and Solving Routing Problems on Quantum Computers", Submitted for publication., 2020.

[S8] D. A. Liñán, **D. E. Bernal**, L. A. Ricardez-Sandoval, and J. M. Gómez, "Optimal synthesis and design of catalytic distillation columns: A rate-based modeling approach", Under review, 2020.

Awards and Honors

- Mark Dennis Karl Teaching Assistant Award   2019
  Chemical Engineering Department - Carnegie Mellon University

- Cum Laude in Chemical Engineering   2014
  Universidad de los Andes

- Valedictorian   2009
  Gimnasio Británico

- First place in the Colombian Physics Olympiad, Superior level   2007
  Universidad Antonio Nariño

Fellowships and Scholarships

- NSF Supplement Award 2038247 Enabling Quantum Computing Platform access with Amazon Web Services   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 Program Award   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

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

- • Fellowship for Masters Degree in Chemical Engineering   2014
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

SERVICE

Peer Reviewing Activities

- – Mathematical Programming   2020
- – Computers & Chemical Engineering   2020
- – Journal of Global Optimization   2019–2020
- – Optimization & Engineering   2019–2020
- – Chemical Engineering Journal   2019
- – American Control Conference   2020

Mentoring at Carnegie Mellon University

- – M.Sc. students Research (Haokun Yang and Yunshan Liu)
- – Undergraduate students Honors Research (Felicity Gong, Rahul Joglekar, Saeed Syed, and Zhifei Yuliu)

Mentoring at Universidad de los Andes

- – Undergraduate students Thesis (Paola Cristancho and Hugo Cuellar)

Membership in Professional Societies

- – American Institute of Chemical Engineering (AIChE)   2014–Current
- – Institute for Operations Research and Management Science (INFORMS)   2017–Current
- – Pittsburgh Quantum Institute (PQI)   2019–Current

Membership in Student Organizations at Carnegie Mellon University

- – Latino Graduate Student Association (LGSA)
- – Society of Hispanic Professional Engineers (SHPE) chapter
- – Spanish And Latin Association (SALSA)
- – INFORMS Student Chapter

- • Liaison of the CMU Quantum Computing group for the Pittsburgh Quantum Institute (PQI)   2019–Current
- • Representative of Chemical Engineering in the CMU INFORMS student chapter   2017–Current
- • Conference chair and organizer of YinzOR Student Conference   2017
- • Session chair at INFORMS Annual Meeting   2019
- • SHPE Annual Meeting CMU College of Engineering Graduate Student Recruiting Volunteer   2020

Extra Courses

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

	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				

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