# CHRISTODOULOS A. FLOUDAS

*1959–2016*

Elected in 2011

*"For contributions to theory, methods, and applications of global optimization in process systems engineering, computational chemistry, and molecular biology."*

BY IGNACIO GROSSMANN

CHRISTODOULOS ACHILLEUS FLOUDAS died August 14, 2016, of a heart attack while vacationing in Greece. He was a highly respected world leader who set very high standards, goals, and challenges in research. The mathematical optimization and process systems engineering communities were deeply shocked at his loss since he was only 56 years old and at the pinnacle of his brilliant professional career.

He was born August 31, 1959, in Ioannina, Greece. After earning his diploma in chemical engineering at the Aristotle University of Thessaloniki in 1982, he came to the United States to continue his education.

I was extremely fortunate to have had Chris Floudas as a PhD student at Carnegie Mellon, where he earned his degree in 1986. He was a truly outstanding student who showed great passion for and devotion to his research. The main paper of his PhD work on automatic synthesis of heat exchanger networks was based on a novel nonlinear programming model and established him as an important contributor in the area.[1] The work enabled network designs to be obtained by optimizing superstructures that contained all the alternative topologies

[1] Floudas CA, Ciric AR, Grossmann IE. 1986. Automatic synthesis of optimum heat exchanger network configurations. *AIChE Journal* 32:276.

(series, parallel, and combinations thereof) for the minimum number of stream matches and minimum energy cost. Chris also extended this work to synthesize flexible heat exchanger networks with uncertain flows and inlet temperatures.

Chris had an exceptional career, first at Princeton (1986–2015), where he became the Stephen C. Macaleer '63 Professor in Engineering and Applied Science, and then at Texas A&M (2015–16), where he was director of the Energy Institute and the Erle Nye '59 Chair Professor for Engineering Excellence.

One of his major contributions was the development of global optimization algorithms. Initially, the most notable was the $\alpha$BB algorithm, which can be used to rigorously find global optima in nonlinear and mixed-integer nonlinear programs.[2] This research, with his students Claire Adjiman, Ioannis Androulakis, and Costas Maranas, is recognized as pioneering in the field of global optimization because of the wide class of functions and constraints it can handle (e.g., bilinear, trilinear, concave, linear fractional, and general twice-differentiable).

The key idea in the $\alpha$BB algorithm was the construction of a converging sequence of upper and lower bounds on the global minimum through the convex relaxation of the original problem. This relaxation is obtained by replacing all nonconvex terms of special structure—bilinear, trilinear, fractional, fractional trilinear, univariate concave—with customized tight convex lower bounding functions and by selecting some suitable value of $\alpha$ to generate valid convex underestimators for nonconvex terms of generic structure. A crucial step was in the use of interval arithmetic on the Hessian matrix or the characteristic polynomial of the function being investigated. These theoretical ideas were implemented using a number of rules for branching variable selection and variable bound updates. The algorithm was successfully tested on a set of challenging test problems, mostly from chemical engineering.

[2] Androulakis IP, Maranas CD, Floudas CA. 1995. $\alpha$BB: A global optimization method for general constrained nonconvex problems. *Journal of Global Optimization* 7(4):337–63.

His more recent accomplishments in global optimization, with his PhD student Ruth Misener, resulted in the development of the global optimization codes GloMIQO[3] and ANTIGONE.[4] The former is for solving mixed-integer quadratic programming problems and has, for instance, been applied successfully to the classic pooling problems that arise in the petroleum industry. ANTIGONE can handle general algebraic nonconvex mixed-integer nonlinear programming models.

The key ideas were the development of the facets of low-dimensional ($n \leq 3$) edge-concave aggregations dominating the termwise relaxation of the mixed-integer quadratically constrained quadratic program (MIQCQP) at every node of a branch-and-bound tree.[5] Concave multivariable terms and sparsely distributed bilinear terms that do not participate in connected edge-concave aggregations were handled through piecewise-linear relaxations. The major algorithmic components of GloMIQO involved reformulating user input, detecting special structure including convexity and edge-concavity, generating tight convex relaxations, partitioning the search space, bounding the variables, and finding good feasible solutions. GloMIQO was extensively tested on 400 test problems of varying size and structure, including general nonconvex terms. The structure of ANTIGONE was based on the previous MIQCQP and mixed-integer signomial optimization computational frameworks. ANTIGONE was tested on 2500 test problems from standard libraries and performed competitively with codes such as BARON, Couenne, and SCIP.

Chris Floudas also made outstanding contributions in the area of batch scheduling, where his work with Marianthi

[3] Misener R, Floudas CA. 2013. GloMIQO: Global mixed-integer quadratic optimizer. *Journal of Global Optimization* 57(1):3–50.

[4] Misener R, Floudas CA. 2014. ANTIGONE: Algorithms for coNTinuous / Integer Global Optimization of Nonlinear Equations. *Journal of Global Optimization* 59(2–3):503–26.

[5] Misener R, Floudas CA. 2012. Global optimization of mixed-integer quadratically-constrained quadratic programs (MIQCQP) through piecewise-linear and edge-concave relaxations. *Mathematical Programming* 136:155–82.

Ierapetritou introduced a novel mathematical formulation for scheduling problems for batch processes with general network structure.[6] That work introduced a novel mixed-integer linear programming model based on a continuous time representation, whereas earlier work was based on the less rigorous discrete time representation.

Chris also did very fine work in areas of synthesis of reactor networks and separation systems. His work has had industrial impact as it has been applied by companies such as Shell, Aspen Technology, BASF, and Atofina Chemicals.

In computational biology Chris introduced a first-principles structure prediction method, ASTRO-FOLD, for helical and beta-sheet topology; invented new methods for NMR structure refinement based on atomistic modeling; and pioneered de novo design strategies for peptides and proteins. His first-principles approach to the latter led to the design of an inhibitor with 45-fold improvement over compstatin, the best-known complement inhibitor; Phase I clinical trials were successfully completed by Potentia Pharmaceuticals for age-related macular degeneration.

More recently, he developed very-large-scale supply chain models for hybrid feedstock for energy for converting coal, biomass, and natural gas to gasoline, diesel, and kerosene. This work, based on multiscale modeling and incorporating materials considerations for the various energy technologies,[7] received a great deal of attention as it addresses the US supply chain. It was also to a large extent the basis for his appointment as director of the Energy Institute at Texas A&M.

Chris gave many keynote talks at major international meetings, was prolific in writing papers (over 350 publications), and was the author of two graduate textbooks, *Nonlinear Mixed-Integer Optimization* (Oxford University Press, 1995) and

[6] Ierapetritou MG, Floudas CA. 1998. Effective continuous-time formulation for short-term scheduling. 1. Multipurpose batch processes. *Industrial & Engineering Chemistry Research* 37:4341–59.

[7] Floudas CA, Niziolek AM, Onel O, Matthews LR. 2016. Multi-scale systems engineering for energy and the environment: Challenges and opportunities. *AIChE Journal* 62:602–23.

*Deterministic Global Optimization* (Kluwer Academic Publishers, 2000). He also coedited the *Encyclopedia of Optimization* (with Panos Pardalos; Springer, 2008) and ten monographs/books. His publications have been cited tens of thousands of times.[8]

For his teaching, research, and writing, Chris received numerous awards and honors: the NSF Presidential Young Investigator Award (1988); Engineering Council Teaching Award, Princeton University (1995); Bodossaki Foundation Award in Applied Sciences (1997); Best Paper Award in Computers and Chemical Engineering (1998); AspenTech Excellence in Teaching Award (1999); AIChE Professional Progress Award for Outstanding Progress in Chemical Engineering (2001) and Computing in Chemical Engineering Award (2006); Graduate Mentoring Award, Princeton University (2007); and National Award and Operational Research Gold Medal from the Hellenic Operational Research Society (2013).

He was also elected to the NAE (2011); selected for China's One Thousand Global Experts (2012–15); and elected a SIAM fellow (2013), AIChE fellow (2013), member of the Academy of Medicine, Engineering, and Science of Texas (2015), corresponding member of the Academy of Athens (2015), and fellow of the National Academy of Inventors (2015). He was designated a TAMU Institute for Advanced Study fellow and eminent scholar (2013–14), received an honorary doctorate from Finland's Åbo Akademi University (2014), and was recognized as a Thomson Reuters Highly Cited Researcher (2014 and 2015).

Chris's legacies include the outstanding PhD students and postdocs he advised and mentored who have taken academic positions; they include Claire Adjiman, Peter DiMaggio, Chrysanthos Gounaris, Faruque Hasan, Marianthi Ierapetritou, Nina Lin, Costas Maranas, and Ruth Misener. His students have also been very well received by industry.

Chris Floudas' death is a huge loss to the mathematical optimization and process systems engineering communities.

[8] His publications have been highly cited (42,000 Google Scholar citations and an h-index over 100 as of September 2021).

He was not only a major intellectual leader but also a very good friend. His absence will be felt for many years. The only consolation is to know that his legacy will continue through his students and that his work will inspire new generations of researchers in optimization and process systems.

We offer our deepest sympathy to his wife Fotini and daughter Ismini. Chris will be sorely missed. May he rest in peace.