

RESEARCH PROFILE AND PUBLICATIONS (2005-2018)

Mathematical modelling, simulation, optimization and control of bioprocesses

The main overall objective of this research line is to improve the efficiency of bioprocesses via **systems engineering** methods. These methods are based on a model-driven systemic approach, i.e. they make extensive use of **mathematical models and simulation, optimization and control methods and tools (software)**.

The ultimate goal is to improve the efficiency of these processes and the quality and safety of their products, reducing energy and water consumption and environmental impact.

There are two main blocks of objectives:

1. **methods**: to develop robust and efficient methods and tools (software) for the multi-scale mathematical modeling, **simulation, optimization, monitoring and control of bioprocesses**
2. **applications**: to apply these methods and tools to real processes and systems of clear interest, such as industrial processes of high economic importance (food and biotechnological sectors), and relevant biosystems associated with them (**systems biology of microorganisms; synthetic biology**)

Papers in Journals (2010-2018)

2018

Alonso, A.A.; Bermejo, R.; Pájaro, M.; Vázquez, C. 2018. Numerical analysis of a method for a partial integro-differential equation model in regulatory gene networks. *Mathematical Models and Methods in Applied Sciences*, 28 (10): 2069-2095. DOI: 10.1142/S0218202518500495

Alonso, A.A.; Otero-Muras, I.; Pájaro, M. 2018. Routes to Multiple Equilibria for Mass-Action Kinetic Systems. *Complexity* 2018: 3912627. DOI: 10.1155/2018/3912627

Bandiera, L.; Hou, Z.; Kothamachu, V.B.; Balsa-Canto, E.; Swain, P.S.; Menolascina, F. 2018. On-line optimal input design increases the efficiency and accuracy of the modelling of an inducible synthetic promoter. *Processes*, 6(9): 148. DOI: 10.3390/pr6090148

García, M.R.; Cabo, M.L. 2018. Optimization of E. coli inactivation by benzalkonium chloride reveals the importance of quantifying the inoculum effect on chemical disinfection. *Frontiers in Microbiology*. DOI: 10.3389/fmicb.2018.01259

García, M.R.; Vázquez, J.A.; Teixeira, I.G.; Alonso, A.A. 2018. Stochastic individual-based modeling of bacterial growth and division using flow cytometry. *Frontiers in Microbiology*. DOI: 10.3389/fmicb.2017.02626

- Gonzalez, P., Martinez, X. C. P., Doallo, R., & Banga, J.R. (2018) Implementing cloud-based parallel metaheuristics: an overview. *Journal of Computer Science and Technology*, 18(03):e26-e26. DOI: 10.24215/16666038.18.e26
- González, P., Penas, D.R., Pardo, X.C., Banga, J.R., Doallo, R. 2018. Multimethod optimization in the cloud: A case-study in systems biology modelling. *Concurrency Computation*, 30 (12): e4488. DOI: 10.1002/cpe.4488
- Henriques, D.; Alonso-del-Real, J.; Querol, A.; Balsa-Canto, E. 2018. *Saccharomyces cerevisiae* and *S. kudriavzevii* synthetic wine fermentation performance dissected by predictive modeling. *Frontiers in Microbiology*, 2018 (9): 88. DOI: 10.3389/fmicb.2018.00088
- Le, T.T.Y.; García, M.R.; Nachev, M.; Grabner, D.; Balsa-Canto, E.; Hendriks, A.J.; Sures, B.. 2018. Development of a PBPK Model for Silver Accumulation in Chub Infected with Acanthocephalan Parasites. *Environmental Science and Technology* 52 (21): 12514-12525. DOI: 10.1021/acs.est.8b04022
- Ligon, T.S.; Fröhlich, F.; Chis, O.T.; Banga, J.R.; Balsa-Canto, E.; Hasenauer, J.. 2018. GenSSI 2.0: Multi-experiment structural identifiability analysis of SBML models. *Bioinformatics*, 34 (8): 1421-1423. DOI: 10.1093/bioinformatics/btx735
- Lopes, C.; Antelo, L.T.; Franco-Uría, A.; Alonso, A.A.; Pérez-Martín, R.. 2018. Chitin production from crustacean biomass: Sustainability assessment of chemical and enzymatic processes. *Journal of Cleaner Production*, 172: 4140-4151. DOI: 10.1016/j.jclepro.2017.01.082
- Méndez-González, J.M.; Otero-Muras, I. 2018. Multistability in a prion replication interconnected cell reaction network. *IFAC-PapersOnLine*, 51 (19): 62-63. DOI: 10.1016/j.ifacol.2018.09.043
- Otero-Muras, I.; Banga, J.R.. 2018. Mixed Integer Multiobjective Optimization Approaches for Systems and Synthetic Biology. *IFAC-PapersOnLine*, 51 (19): 58-61. DOI: 10.1016/j.ifacol.2018.09.042
- Otero-Muras, I.; Banga, J.R. 2018. Optimization-based prediction of fold bifurcations in nonlinear ODE models. *IFAC-PapersOnLine*, 51 (15): 485-490. DOI: 10.1016/j.ifacol.2018.09.192
- Pájaro, M.; Otero-Muras, I.; Vázquez, C.; Alonso, A.A. 2018. Efficient simulation of stochastic gene regulatory networks. *IFAC-PapersOnLine*, 51 (19): 84-85. DOI: 10.1016/j.ifacol.2018.09.033
- Pájaro, M.; Otero-Muras, I.; Vázquez, C.; Alonso, A.A. 2018. SELANSI: A toolbox for simulation of stochastic gene regulatory networks. *Bioinformatics*, 34 (5): 893-895. DOI: 10.1093/bioinformatics/btx645
- Pitt, J.A.; Gomoescu, L.; Pantelides, C.C.; Chachuat, B.; Banga, J.R. 2018. Critical Assessment of Parameter Estimation Methods in Models of Biological Oscillators. *IFAC-PapersOnLine*, 51 (19): 72-75. DOI: 10.1016/j.ifacol.2018.09.040
- Teijeiro, D.; Pardo, X.C.; González, P.; Banga, J.R.; Doallo, R. 2018. Towards cloud-based parallel metaheuristics: A case study in computational biology with Differential Evolution and Spark. *International Journal of High Performance Computing Applications*, 32 (5): 693-705. DOI: 10.1177/1094342016679011
- Tsiantis, N.; Balsa-Canto, E.; Banga, J.R. 2018. Optimality and identification of dynamic models in systems biology: An inverse optimal control framework. *Bioinformatics*, 34 (14): 2433-2440. DOI: 10.1093/bioinformatics/bty139

Vázquez, J.A., Fraguas, J., Novoa-Carvallal, R., Reis, R.L., Antelo, L.T., Pérez-Martín, R.I., Valcarcel, J. 2018. Isolation and chemical characterization of chondroitin sulfate from cartilage by-products of blackmouth catshark (*Galeus melastomus*). *Marine Drugs*, 16 (10), art. no. 344. DOI: 10.3390/md16100344. Open Access.

Vázquez, J.A., Ramos, P., Valcarcel, J., Antelo, L.T., Novoa-Carballal, R., Reis, R.L., Pérez-Martín, R.I. 2018. An integral and sustainable valorisation strategy of squid pen by-products. *Journal of Cleaner Production*, 201:207-218. DOI: 10.1016/j.jclepro.2018.07.316

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Vilas, C.; Arias-Méndez, A.; García, M.R.; Alonso, A.A.; Balsa-Canto, E.. 2018. Towards predictive food process models: A protocol for parameter estimation. *Critical Reviews in Food Science and Nutrition*, 58 (3): 436-449. DOI: 10.1080/10408398.2016.1186591

Villaverde, A.F.; Becker, K.; Banga, J.R. 2018. PREMER: A Tool to Infer Biological Networks. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 15 (4): 1193-1202. DOI: 10.1109/TCBB.2017.2758786

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BALSA-CANTO E, LÓPEZ-NÚÑEZ A, VÁZQUEZ C. 2017. Numerical methods for a nonlinear reaction-diffusion system modelling a batch culture of biofilm *Applied Mathematical Modelling* 18:164-179 DOI: 10.1016/j.apm.2016.08.020.

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PENAS DR, GONZÁLEZ P, EGEE JA, DOALLO R, BANGA, JR. 2017. Parameter estimation in large-scale systems biology models: A parallel and self-adaptive cooperative strategy. *BMC Bioinformatics* 18(1) DOI: 10.1186/s12859-016-1452-4.

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VILAS C, ALONSO AA, HERRERA J.R, GARCÍA-BLANCO A, GARCÍA M.R. 2017. A model for the biochemical degradation of inosine monophosphate in hake (*Merluccius merluccius*). *Journal of Food Engineering* 200:95-101 DOI: 10.1016/j.jfoodeng.2016.12.016

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