Results of computer simulations of inter-microbial metabolic exchange.

Website: https://www.bco-dmo.org/dataset/806874
Data Type: model results
Version: 1
Version Date: 2022-02-03

Project
» Microbial ecosystems in silico, in the lab and in the field: understanding interactions between abundant marine bacterial taxa (HADFBA)

Contributors	Affiliation	Role
Segre, Daniel	Boston University (BU)	Principal Investigator
Sher, Daniel	University of Haifa	Co-Principal Investigator
Biddle, Mathew	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager
Soenen, Karen	Woods Hole Oceanographic Institution (WHOI BCO-DMO)	BCO-DMO Data Manager

Abstract
Results of computer simulations of inter-microbial metabolic exchange. The Zipped directory contains scripts and computationally generated predictions of growth phenotypes of pairs of bacteria under different growth conditions.

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Dataset Description

The Zipped directory contains scripts and computationally generated predictions of growth phenotypes of pairs of bacteria under different growth conditions.

The results from all growth simulations (1,051,596 simulations of two organisms with two carbon sources, with and without oxygen) are contained in the MATLAB structure 'MData.' Results are also provided in CSV format in 'MData.csv.zip.'

MData contains the following fields:

- aer and anaer: Data structures containing the following results for the simulations with and without oxygen, respectively:

- allGrewAlone: Binary vectors denoting whether or not both organisms grew in the first iteration of the algorithm.

- allGrewCross: Binary vectors denoting whether or not both organisms grew in the last iteration of the algorithm (after cross-feeding).

- expansions: Numerical vector detailing the number of medium expansions that occured in each simulation

- secMetCountsAlone: Numerical vector containing the number of metabolites secreted at the first iteration of each simulation.

- secMetCountsCross: Numerical vector containing the number of metabolites secreted at the last iteration of each simulation.

- sharedMedium: Cell array detailing the minimal medium composition.

- sub: Sparse binary double matrix detailing phenotypic information for the first (subject) organism in each simulation. Rows are simulations, column identities are contained in MData.col (Data given as row, column, value pairs in CSV version).

- par: Sparse binary double matrix detailing phenotypic information for the second (partner) organism in each simulation. Rows are simulations, column identities are contained in MData.col (Data given as row, column, value pairs in CSV version).

- Motifs: Data structure with two fields:

- MotifsGen: Cell array detailing the general interaction type in each simulation (C: commensal, M: mutualistic, N: non-interacting).

- MotifsSp: Cell array detailing the specific interaction motifs in each simulation (detailed in main text).

- col: Data structure defining which columns in the 'sub' and 'par' matrices correspond to phenotypic information (Species: organisms, CSources: carbon sources, absMets: absorbed metabolites corresponding to MData.fullMetList, secMets: secreted metabolites corresponding to MData.fullMetList, O2: oxygen availability, growthAlone: whether the organism grew alone in minimal medium, growthCross: whether the organism grew after cross-feeding).

- fullMetList: Cell array of all extracellular metabolites in all organism models.

- speciesPairCombos: Cell array of organisms used in each of the simulations.

- CSource pair combos: Cell array of carbon sources used in each of the simulations.

The model code is available in as .zip file: https://datadocs.bco-dmo.org/data/302/HADFBA/806874/1/data/CostlessExcha...
These files are also available in the following GitHub repository:
https://github.com/BCODMO/CostlessExchange/tree/v1.0

Data Processing Description

BCO-DMO Processing Notes:

Originally submitted GitHub repository https://github.com/segrelab/CostlessExchange forked to https://github.com/BCODMO/CostlessExchange and tagged with release v1.0 which corresponds with this dataset submission.

The original repository may have continued updates.

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Data Files

File

Results of computer simulations of inter-microbial metabolic exchange

filename: CostlessExchange-1.0.zip

(ZIP Archive (ZIP), 93.37 MB)
MD5:933aa750bddd62f5bd89f9c9061fd65a

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Related Publications

Pacheco, A. R., Moel, M., & Segrè, D. (2019). Costless metabolic secretions as drivers of interspecies interactions in microbial ecosystems. Nature Communications, 10(1). doi:10.1038/s41467-018-07946-9
Results

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Parameters

Parameters for this dataset have not yet been identified

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Project Information

Microbial ecosystems in silico, in the lab and in the field: understanding interactions between abundant marine bacterial taxa (HADFBA)

Coverage: Eastern Mediterranean Sea

Every drop of seawater contains around one million microorganisms (bacteria, small algae and other organisms such as ciliates and diatoms). These marine microbes feed the entire marine ecosystem, modulate global cycles of carbon and other elements, and impact climate. With the advances in genome-sequencing technology, we can now identify the microbes and assess their genetic and metabolic capacities, yet we still cannot deduce from the genomes of these organisms how they will grow - and interact - in nature. The proposed project will tackle this challenge through a tightly integrated combination of mathematical modeling, laboratory experiments and field work in the Eastern Mediterranean, to identify genes and pathways dictating how environmentally-relevant microbes grow and interact in the sea. We will produce genome-scale mathematical models of the metabolism of *Prochlorococcus*, the numerically-dominant photosynthetic bacteria in large swaths of the ocean, and of *Alteromonas*, abundant marine bacteria which make their living by consuming and respiring organic molecules produced by *Prochlorococcus* and other photosynthetic microbes. We will test these models using laboratory cultures of these organisms grown alone and together, and determine to what extent the models and laboratory cultures represent the growth and death of these organisms in the Eastern Mediterranean. This study will be useful for scientists of many disciplines, including not only marine biology, oceanography and ecology but also genetics, medicine and agriculture. Our results will shed light on the dynamics of some of the most common organisms in the world, responsible for the production of up to 20% of the oxygen we breathe. Our collaborative study will foster the development and training of the next generation of marine scientists, and will be used in outreach activities designed to share with high-school students and the general public the excitement of marine research and the need to responsibly utilize and sustain the oceans for the sake of future generations.

The proposed project will tackle the challenge of understanding microbial interactions from the underlying genetic data through a tightly integrated combination of genome scale modeling, laboratory experiments and field work in the Eastern Mediterranean. We aim to identify genomic traits dictating how environmentally-relevant primary producers and heterotrophic bacteria interact. Genome-scale (dynamic flux balance analysis, dFBA) models of *Prochlorococcus* MED4 and of *Alteromonas* HOT1A3 will be produced and calibrated using high-throughput measurements of growth and physiological parameters in laboratory batch cultures, combined with detailed analysis of specific metabolites; The dFBA models will be combined *in-silico* and the results compared to laboratory co-cultures. Model-data discrepancies will provide opportunities to revisit the models, suggesting the mediation of alternative processes such as allelopathy or other types of chemical signaling. Finally, time-series data on the community composition and function during the summer/fall *Prochlorococcus* bloom in the hyper-oligotrophic Eastern Mediterranean, combined with field experiments (microcosms), will provide a test of hypotheses generated in the lab. This study will provide the first detailed "roadmap" linking genomic traits (genes and metabolic pathways) and rate measurements with species interactions in environmentally-relevant marine microbes. Genome-scale models will likely be embedded in a not-so-distant future in global-scale models of the Earth System, and the proposed study will provide a critical stepping-stone towards predicting how marine microbial systems will evolve in a changing world. The strong

human impact on marine ecosystems, and the need for quantitative and predictive understanding of how they will respond to a changing environment, calls for interdisciplinary research and training for the next generation of scientists and decision makers. Models and data generated by our work will be integrated into a novel educational exploration-focused, web- and field-based educational module. This module will introduce key concepts in microbiology, environmental sciences and oceanography to intermediate- and high-school students.

(Note: acronym HADFBA = Heterotroph-Autotroph Dynamic Flux Balance Analysis)

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-1635070

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