A gene-centric approach to integrating environmental genomics and biogeochemical models

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Introduction

Molecular tools are providing profound insights into the composition and function of marine microbial communities. Despite these organisms playing key roles in regulating global geochemical cycles, biogeochemical models typically do not incorporate bacteria and archaea explicitly, nor are such models compatible with nucleic acid or protein sequence data. Here, we present a method for incorporating microbial communities into such models in an effort to provide a detailed mechanistic understanding of marine biogeochemistry, while also exploiting this rapidly growing body of molecular data.

Overview of the functional gene approach

- The microbial community is divided according to metabolism (e.g., hydrogen oxidation, sulphate reduction)
- Functional gene abundances are used as a proxy for associated microbes (e.g., hzo for anammox bacteria)
- Growth & uptake are modelled using Michaelis-Menten kinetics for reactants, nutrients, & inhibitors
- Growth rate is also a linear functional of functional gene abundances
- Growth is coupled to uptake of reactants & nutrients through an empirical thermodynamic relationship
- Growth yields are linearly related to the free energy of metabolisms (Roden & Jin, 2011)
- Metabolic plasticity is included, where growth via one metabolism leads to propagation of genes for another

Figure 1: A cartoon of the functional gene modelling approach for ammonia oxidation. The functional gene amoA is used as a proxy for the abundance of ammonia oxidisers. The reaction converts ammonia and oxygen into nitrite and energy generated by the reaction is converted into growth using an empirical relationship.

Model-data comparisons

- Modelled genes can be expressed both in absolute (# genes L-1) & relative terms (% of genes considered)
- Results are therefore directly comparable to numerous omics data types (e.g., qPCR, assembly)
- It is challenging to include proteinic & transcriptomic data, although initial results are promising (e.g., Fig. 4)

Future work

Parameter problems
- How best to determine parameters for these models since many microbes cannot be cultured?
- Are parameters from analogous systems informative given the wide range of values observed?
- Is parameter fitting a better option?
- Can we circumvent the identifiability problem with biological insight & theory?

Expanding the scope of the approach
- Can similar techniques be employed to study virus-host dynamics?
- Or, do complex interactions & rapid evolution preclude the use of marker genes to track viral populations?

Acknowledgements

This work is funded by Gordon and Betty Moore Foundation Grant GBMF28053 (to G.O.J.) and Grant GBMF32927 (to J.A.H.)

References

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Results

- The model accurately describes the spatial variations observed in chemical species & gene abundances
- Simulations demonstrate that denitrification dominates over anammox in the Arabian Sea
- These results are consistent with experimental studies in the region (Ward et al., 2009)
- Reaction rates in the model are comparable to those measured using isotopic labelling techniques
- Results (not shown) underscore the need for these methods for elucidating cryptic sulphur cycling

Examples

Example #1: Arabian Sea oxygen minimum zone

Oxygen minimum zones (OMZ) represent only 4% of the ocean by volume and yet account for 30-50% of the global marine N2 production. Key questions in OMZs are the relative rates of denitrification and anammox in removing fixed nitrogen from the oceans, as well as how these nitrogen dynamics are affected by cryptic sulphur cycling. While cryptic sulphur cycling is chemically elusive, molecular data provides a means of tracking the associated processes.

- A 1D model is developed that simulates nitrogen cycling across the Arabian Sea OMZ
- Simple parameterisations of transport due to upwelling and turbulent mixing are included in the model
- There are 10 different metabolisms (i.e., functional genes) included in the model & 7 chemical species
- Model results are validated through comparison with chemical and qPCR data from Pitcher et al. (2011)
- Simulations were undertaken to examine the impact of cryptic sulphur cycling on nitrogen dynamics

Example #2: Deep-sea hydrothermal plumes

Hydrothermal vents are oases in the deep ocean that support extensive biological communities. Along mid-ocean ridges, hot fluids rich in reduced chemical species well up from beneath the seafloor and are injected into the cold, oxic water column from vent chimneys, supplying chemolithoautotrophs with an energy source with which to fix carbon. These natural perturbations to the deep-sea microbiome provide an excellent opportunity to study the dynamics of marine microbial communities.

- A physico-biogeochemical model simulates the deep-sea microbial response to hydrothermal plumes
- 7 chemosynthetic metabolisms and 10 chemical species are simulated
- A fluid dynamics model prescribes transport within the plume & entrainment of ambient seawater
- Assembly data prescribe microbial communities at the base of the plume and in ambient seawater

Results

- Simulations show all metabolisms, except for one, adopt a high-affinity-low-growth rate strategy
- These kinetics are to be expected for deep sea communities, as reactant concentrations are low
- Hydrogen oxidation shows the opposite trend, adopting a high growth rate-low affinity strategy
- This is to be expected as the hydrogenase modelled is associated with high H2 production
- Results suggest that ecological strategies can be inferred by fitting model results to omics data
- Simulations exhibit a wide range of possible outcomes due to variations in kinetic parameters

Figures

Figure 2 (left): The location of the field site, marked with a star, in the Arabian Sea (latitude 25°S, longitude 90°E). Figure 2 (right): A schematic of an oxygen minimum zone. Organic matter exported from productive surface waters is decomposed as it sinks, consuming oxygen. In some regions, oxygen concentrations drop to zero below a certain depth. The model accurately describes the spatial variations observed in chemical species & gene abundances (not shown) underscore the need for these methods for elucidating cryptic sulphur cycling.

Figure 3: Absolute gene abundances (qPCR) in the Arabian Sea oxygen minimum zone. Growth yields are linearly related to the free energy of metabolisms (Roden & Jin, 2011). Growth energies are converted into carbon using an empirical relationship. These kinetics are to be expected of deep sea communities, as reactant concentrations are low.

Figure 5: Simulations exhibit a wide range of possible outcomes due to variations in kinetic parameters.

Figure 6: A comparison of model results and observations. There are 7 pathways: aerobic oxidation of sulphur (thiosulfate, elemental sulphur, hydrogen sulphide), nitrile, hydrogen, ammonia, & methane. The model was run with a wide range of kinetic parameters and those that produce the best fit to the data were determined. A simple ecological trade-off was adopted for these kinetic: affinity for reactants is inversely related to growth rate.