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Agent-based modelling of Earth's earliest ecosystems

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**NATURAL
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**Quantifying and
Understanding
the Earth System**



Outline

- Why agent-based modelling?
- A simple example: adaptive dynamics and r/K-selection
- A geological setting
 - The Archean and the emergence of oxygenic photosynthesis
 - The Great Oxidation Event
- A simple model to investigate the emergence of oxygenic photosynthesis.
 - Negative fractionations in $\delta^{13}\text{C}_{\text{org}}$ *ca* 2.7 Ga
- Conclusions



Why agent-based modelling?

- Population heterogeneity
 - The importance of intra-population variability, and its impact on system level properties
 - Bridging the gap between population level model outputs and individual observations
- Emergence
 - Aggregating individual behaviour – all modelling, at some point, needs representative agents to emerge. The key is to get the right representatives for the right reasons.
 - “Reductionism” does not necessarily imply “constructionism” *Anderson (1972)*
 - Levels of representation
- The absence of a continuum
 - Discreet objects/events and the breaking of the continuum hypothesis
- Adaptive/evolutionary processes



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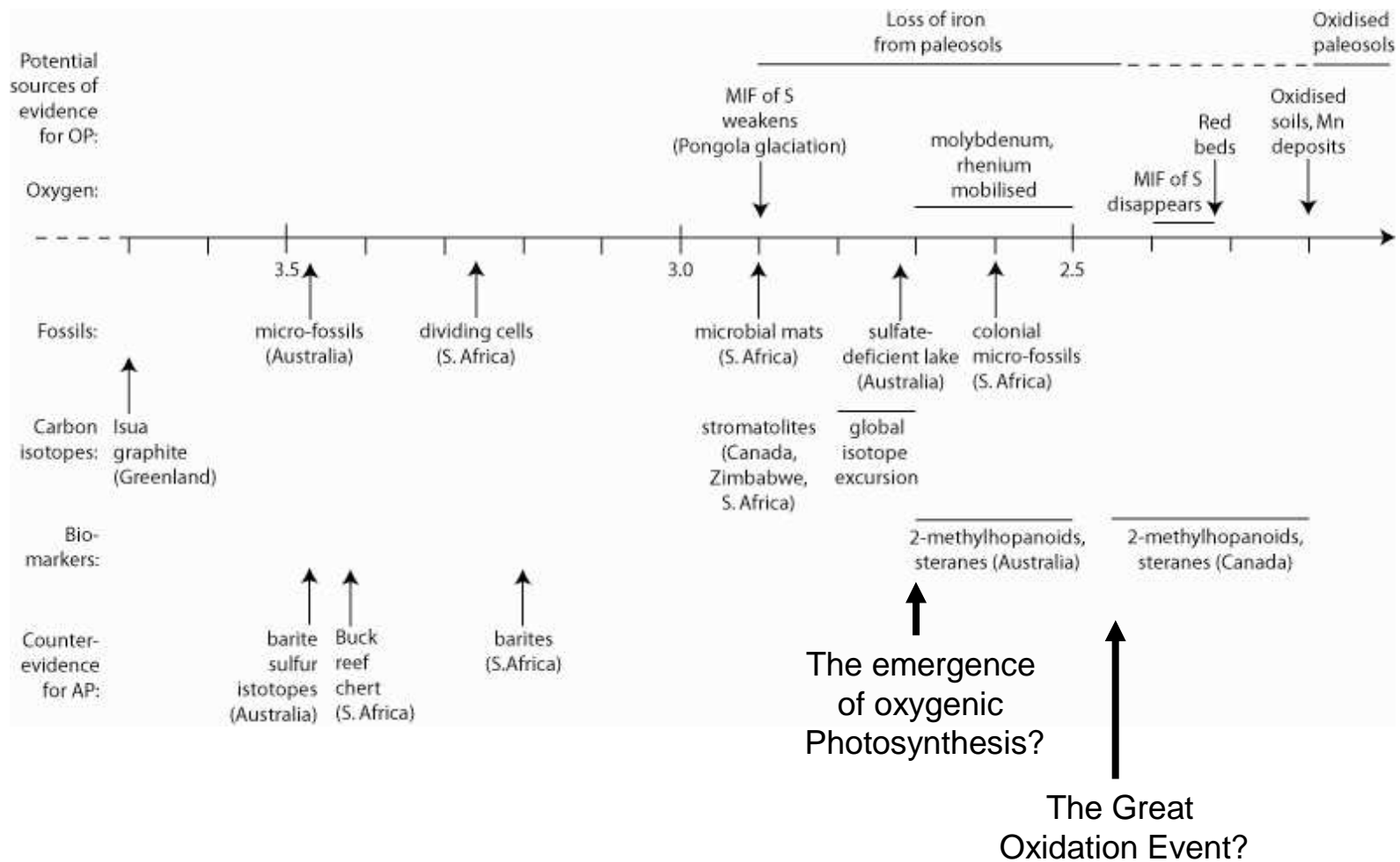
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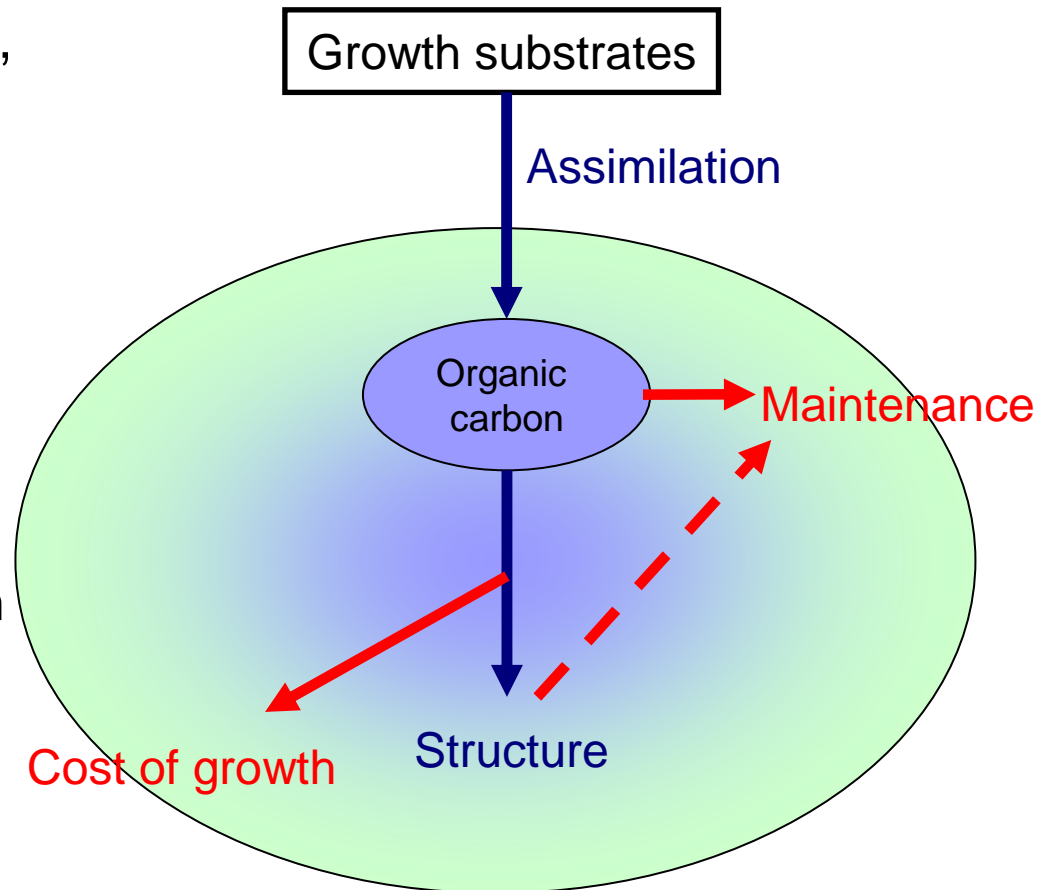
Earth's earliest ecosystems: The Archean



Model design

- Focus on the cycling of carbon, hydrogen and oxygen within a simple box model
- Locations are seeded with three organism types:
 - Chemoheterotrophs
 - Aerobic methanotrophs
 - Methanogens
- We use a Monod-type growth model with an explicit inclusion of metabolic costs

$$\frac{dB}{dt} = Y_{GE} \frac{V_{\max} [X]}{k_m + [X]} - mB$$

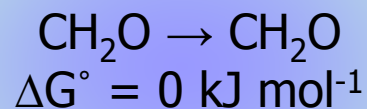


Model design

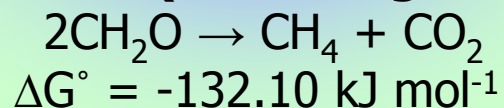
- Net primary production through oxygenic photosynthesis is prescribed

Methanogen (Syntrophy)

Assimilation:

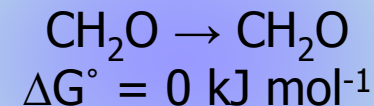


Catabolic (methanogenesis):

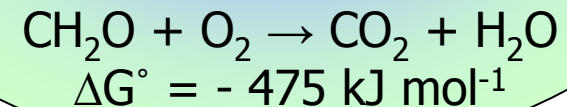


Chemoheterotroph

Assimilation:

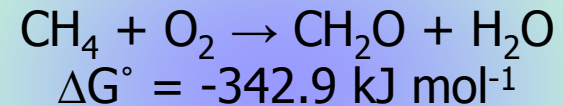


Catabolic (aerobic respiration):

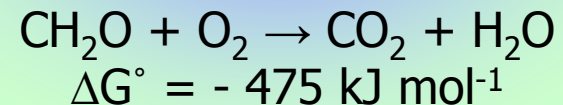


Methanotroph

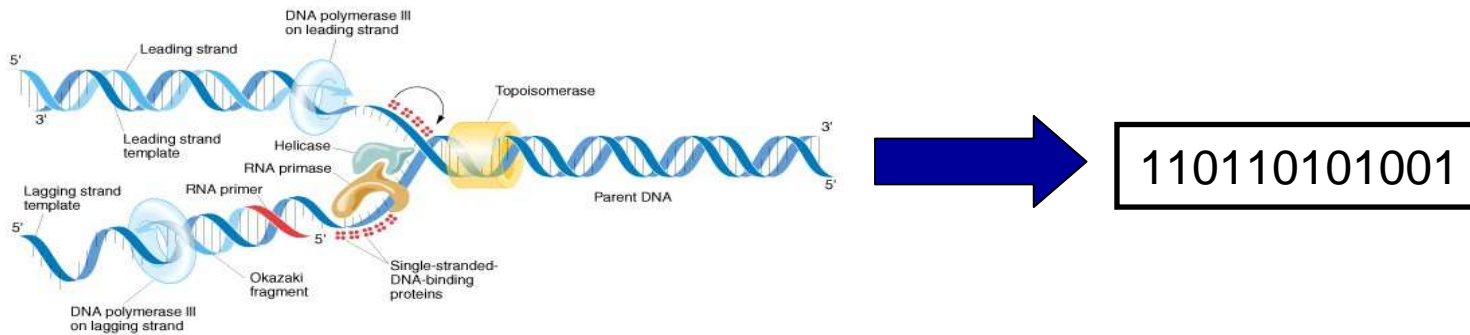
Assimilation:



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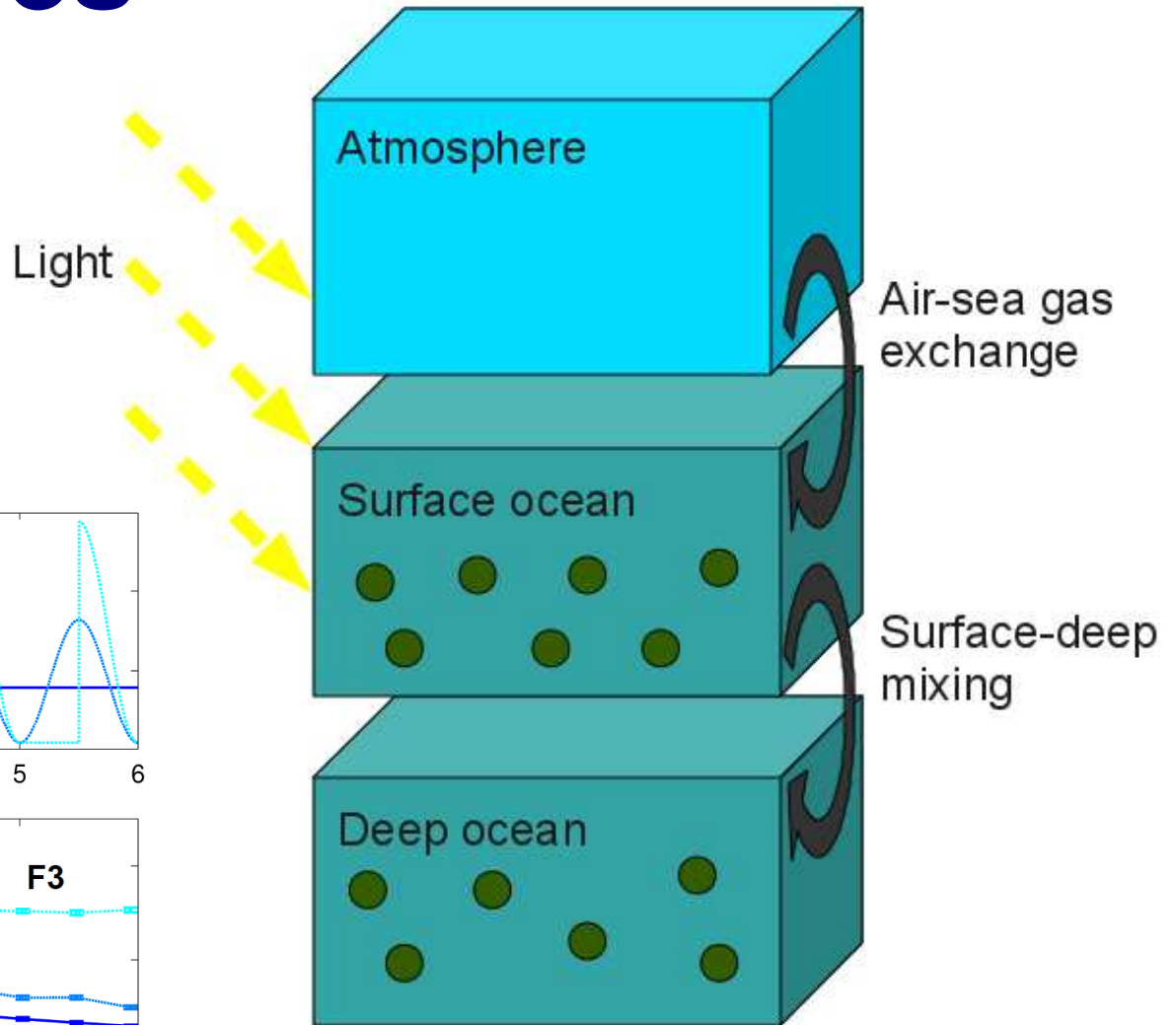
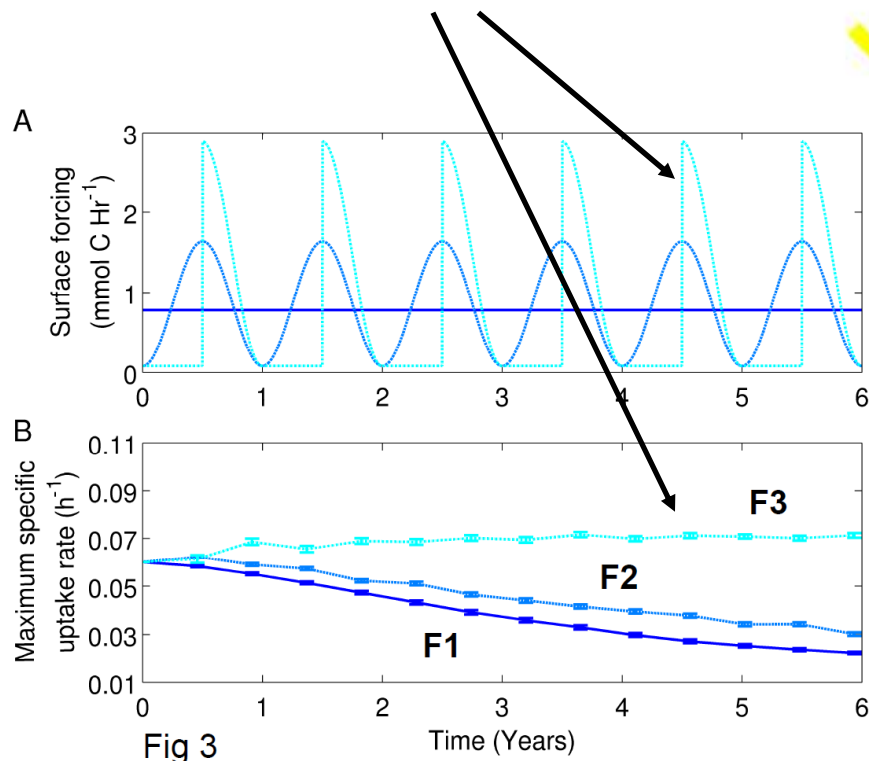
Microbial genome



- Growth rates and resource sensitivities are all genetically defined.
- During reproduction, point mutations may occur with a small probability.
- A simple trade-off between maximum assimilation rate and resource sensitivity is implemented, allowing for the emergence of r/K-strategies.

r/K-strategies

- In a three box configuration, under variable forcing, r-strategists emerge

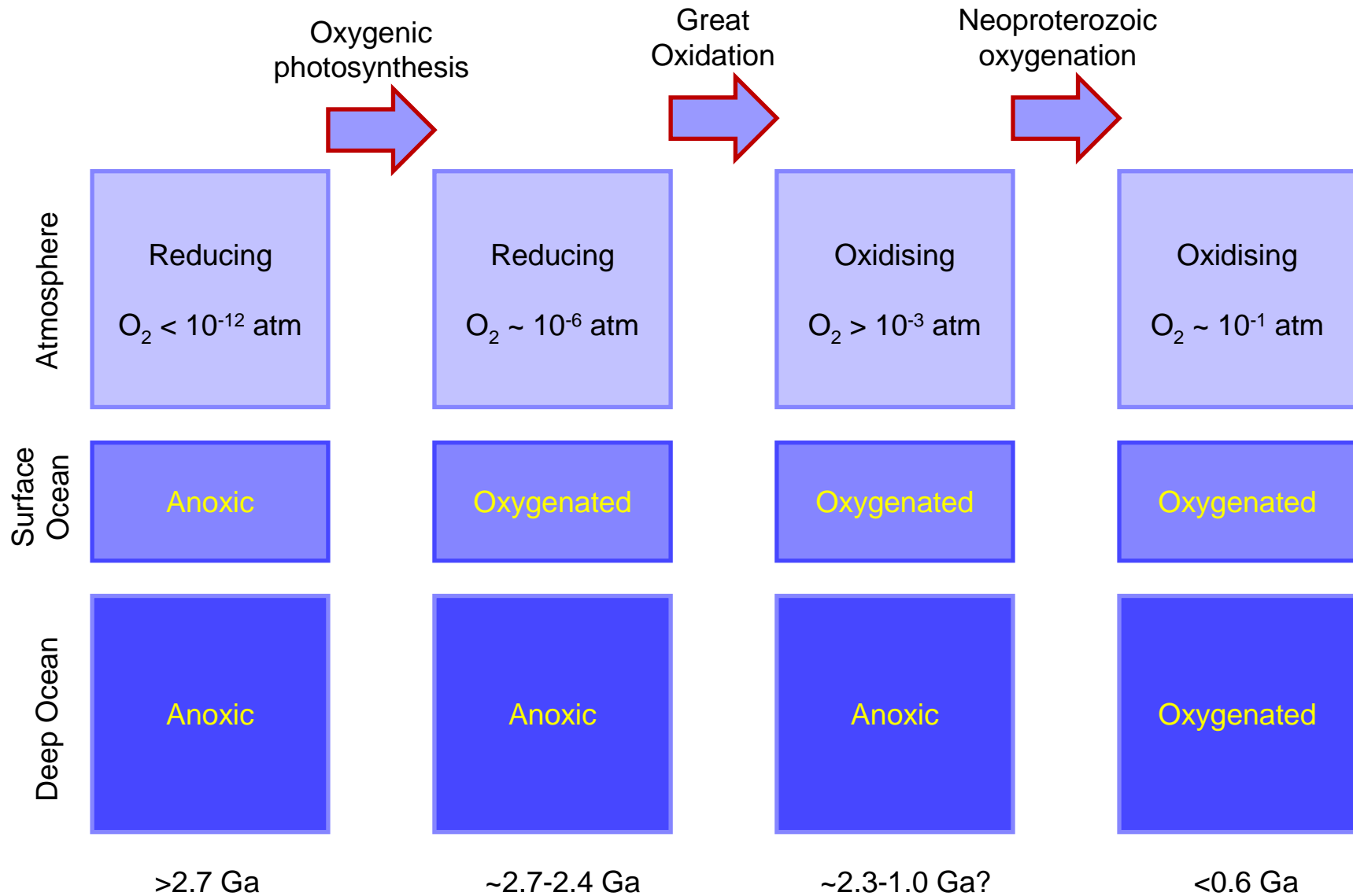
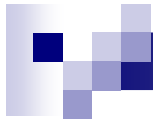


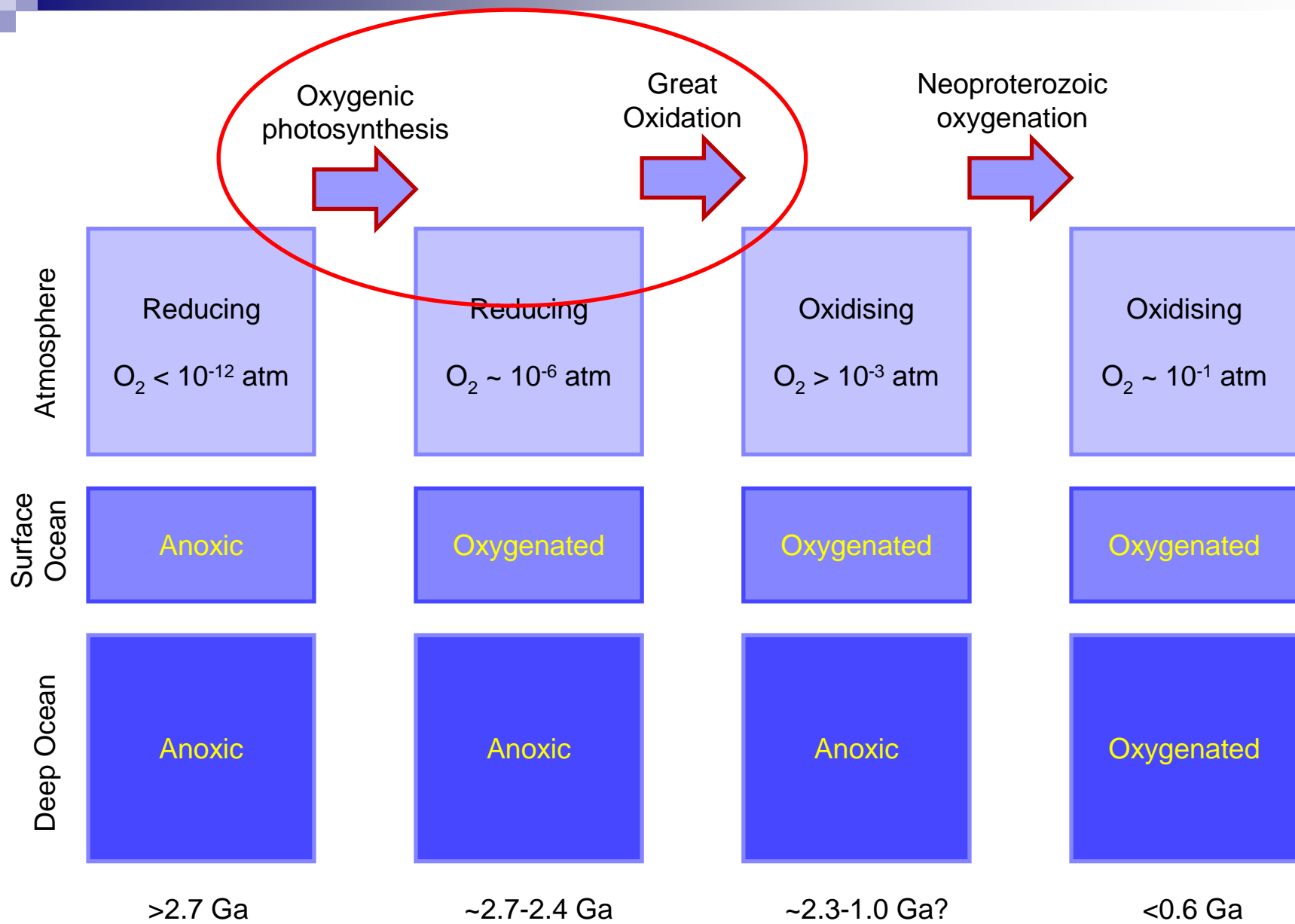
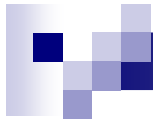
Clark et al submitted (2009)



r/K-strategies

- By incorporating a simple trade-off between maximum assimilation rate and the resource half-saturations constants, one can see different populations of individuals emerge under different forcing conditions.
- Population heterogeneity is incorporated and maintained through mutations.
- Natural selection is observed to operate on model individuals.
- Although the trade-off is rather crude, the potential exists for more detailed agent-based models to inform population level models.

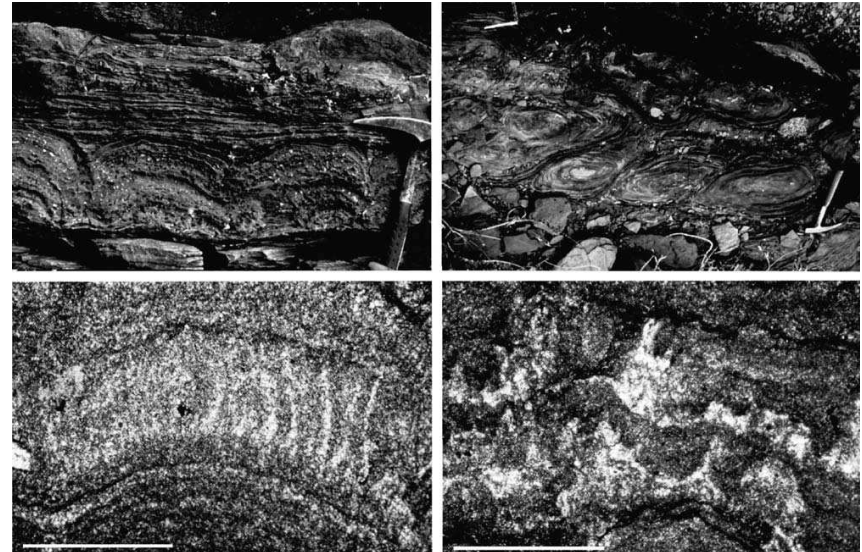




The emergence of oxygenic photosynthesis

■ Stromatolites

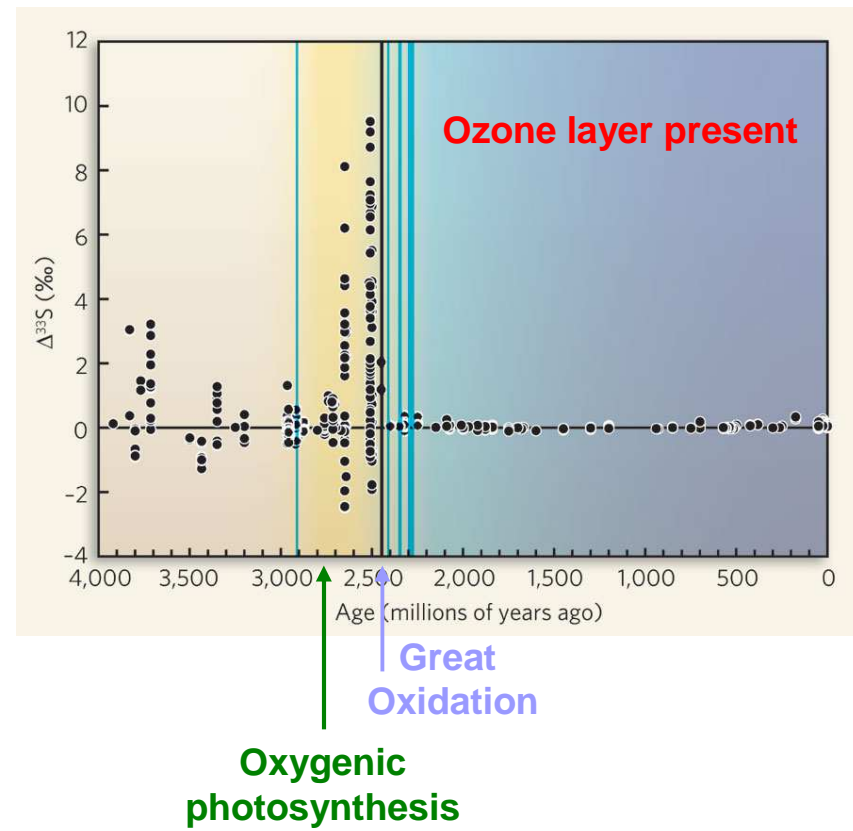
- Formed in modern settings by cyanobacteria (e.g., Australia)
- Later samples strongly suggest the presence of oxygenic phototrophs ca 2.7 Ga, although anoxygenic photosynthesis cannot be fully ruled out.



Lacustrine stromatolites from the ca 2.72 Ga Tumbiana formation, Pilbara, Australia

The emergence of oxygenic photosynthesis

- Evidence for free oxygen
 - Large negative excursions in $\delta^{13}\text{C}_{\text{org}}$ (2.7 Ga)
 - Banded iron formations (<2.4 Ga)
 - An enrichment in redox-sensitive transition metals Mo and Re, evidence for oxidative weathering (2.5-2.7 Ga)
 - MIF of sulphur isotopes, $\text{O}_2 < 10^{-5}$ PAL (~2.45 Ga)

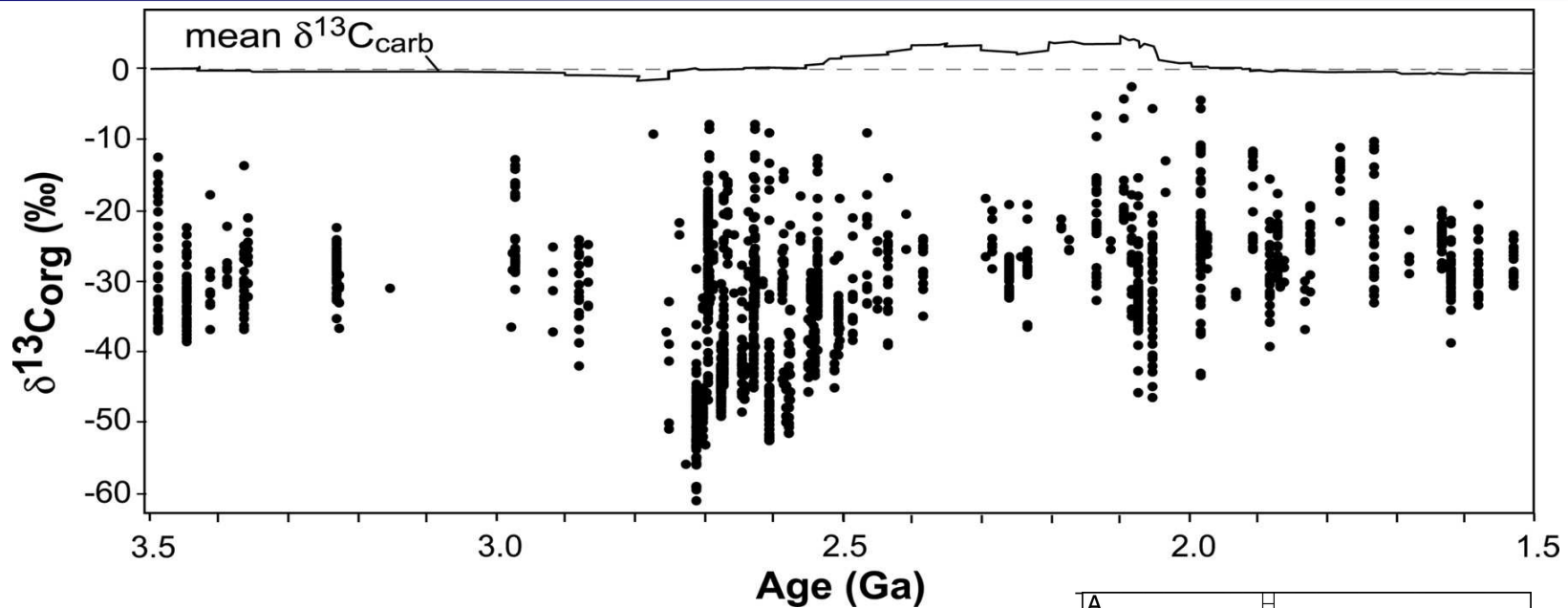


Zahnle, Nature (2008)

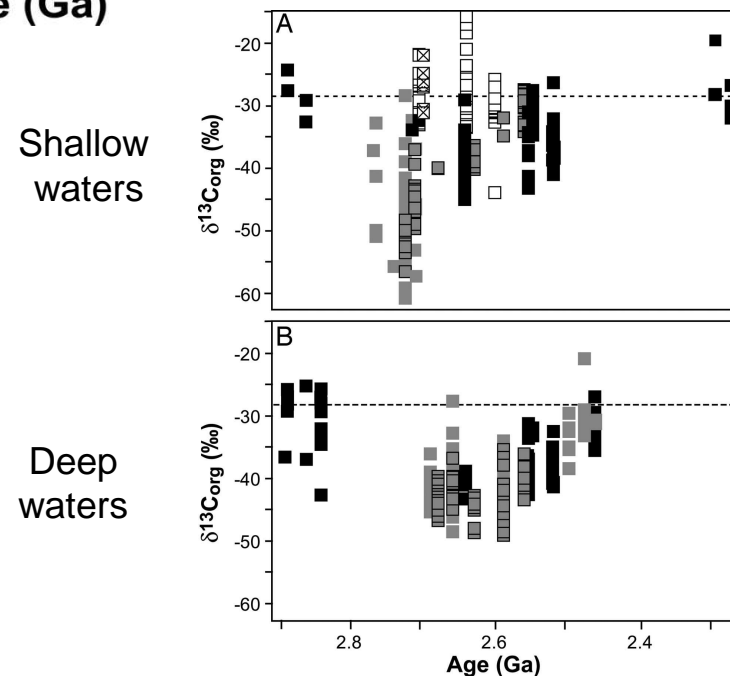


The emergence of oxygenic photosynthesis

- Despite numerous lines of evidence, no one piece conclusively points towards the early emergence of oxygenic photosynthesis
- However, taken together, there is a relatively strong case for it having emerged a significant time before the Great Oxidation Event.
- This said, many still feel that there was no significant delay between the emergence of oxygenic photosynthesis and the oxidation of the atmosphere.



- Negative excursions in $\delta^{13}\text{C}_{\text{org}}$ (2.7 Ga)
 - Methanotrophy producing the most negative $\delta^{13}\text{C}_{\text{org}}$ signal in oxygenated surface waters?
 - Oxygenic photosynthesis had already evolved by 2.7 Ga?





CHAPTER 12

GEOCHEMICAL EVIDENCE BEARING ON THE ORIGIN OF AEROBIOSIS, A SPECULATIVE HYPOTHESIS

By J. M. Hayes

12-1. Introduction

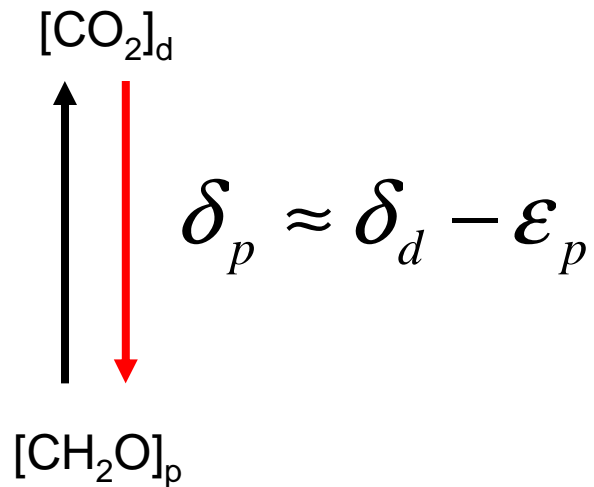
The atmosphere and hydrosphere of the early Archean earth were essentially anoxic; the crust was at that time relatively rich in unoxidized inorganic materials (Chapter 11). An environment without oxygen, the Earth was then a different planet, from the perspective of either the biochemist or geochemist. The paleontological record (Chapters 8 and 9) shows, nevertheless, that life existed on that different planet, and it is widely held that the advent of oxygenic photosynthesis was the singular event that led eventually to our modern environment. The significance and scope of this transition can hardly be overstated, but evidence

12-2. The Carbon Isotopic Record

The isotopic analyses summarized in Figure 7-3 (which presents not only results obtained by the P.P.R.G., but by many previous investigators as well) show that the relative abundance of carbon-13 in sedimentary organic material varies especially widely for about 10^9 years beginning about 2.8 Ga ago. To explore possible explanations for this isotopic fluctuation, it is necessary first to consider the mechanisms by which isotopic abundances are controlled during the biogeochemical cycling of carbon.

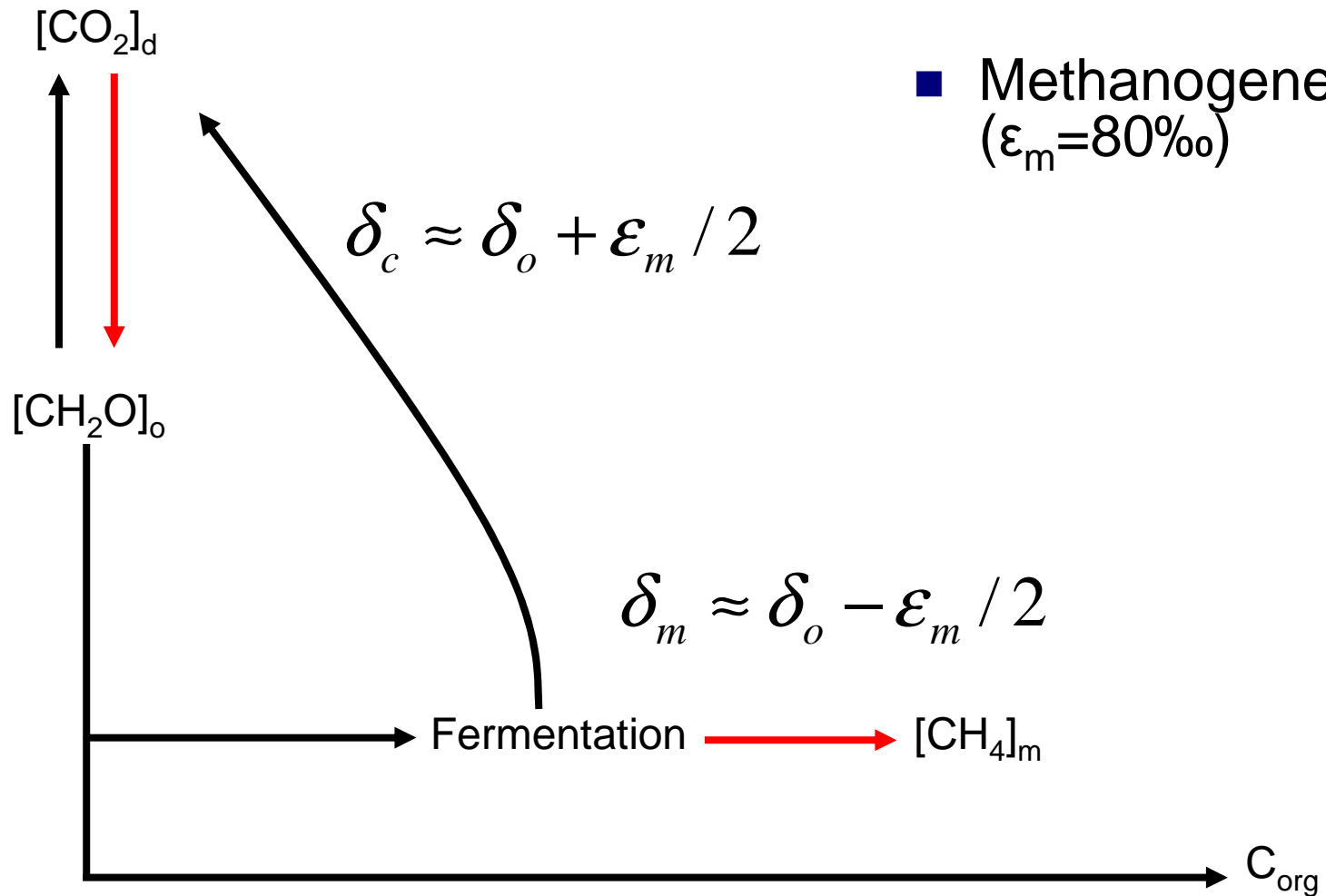
The distribution of carbon isotopes between inorganic and organic carbon pools during ge-

Fractionation effects

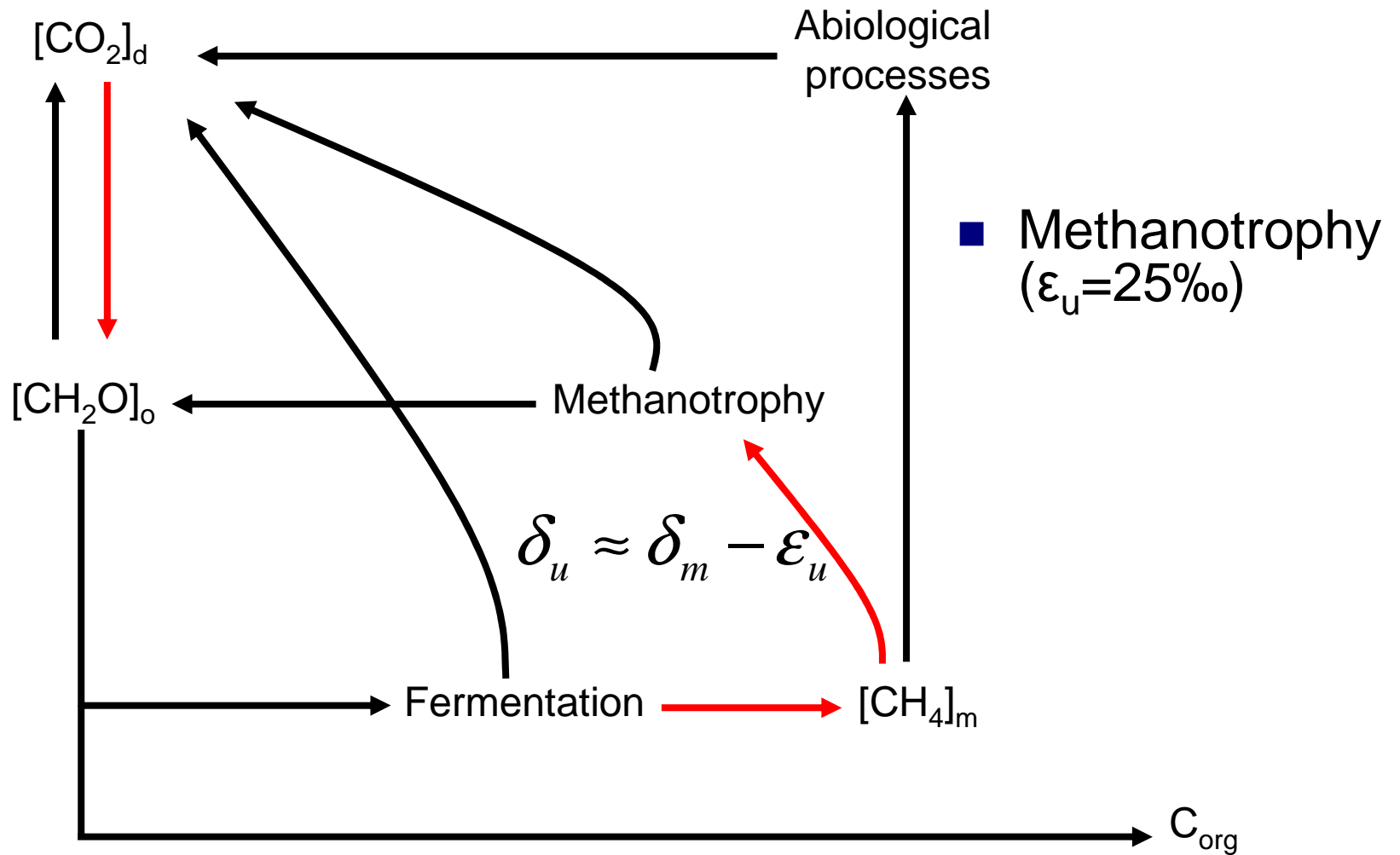


- Oxygenic photosynthesis ($\epsilon_p=30\text{‰}$)

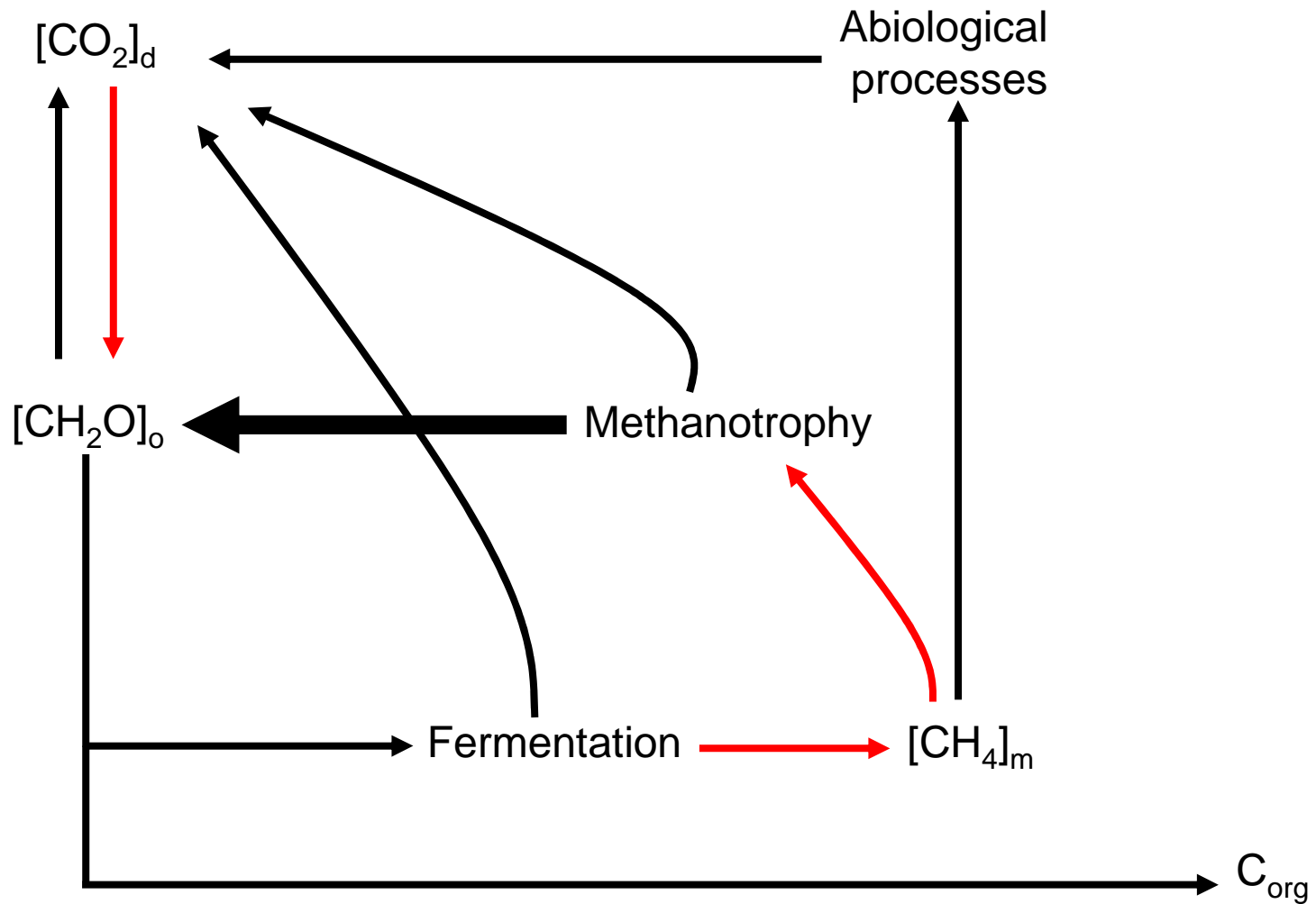
Fractionation effects



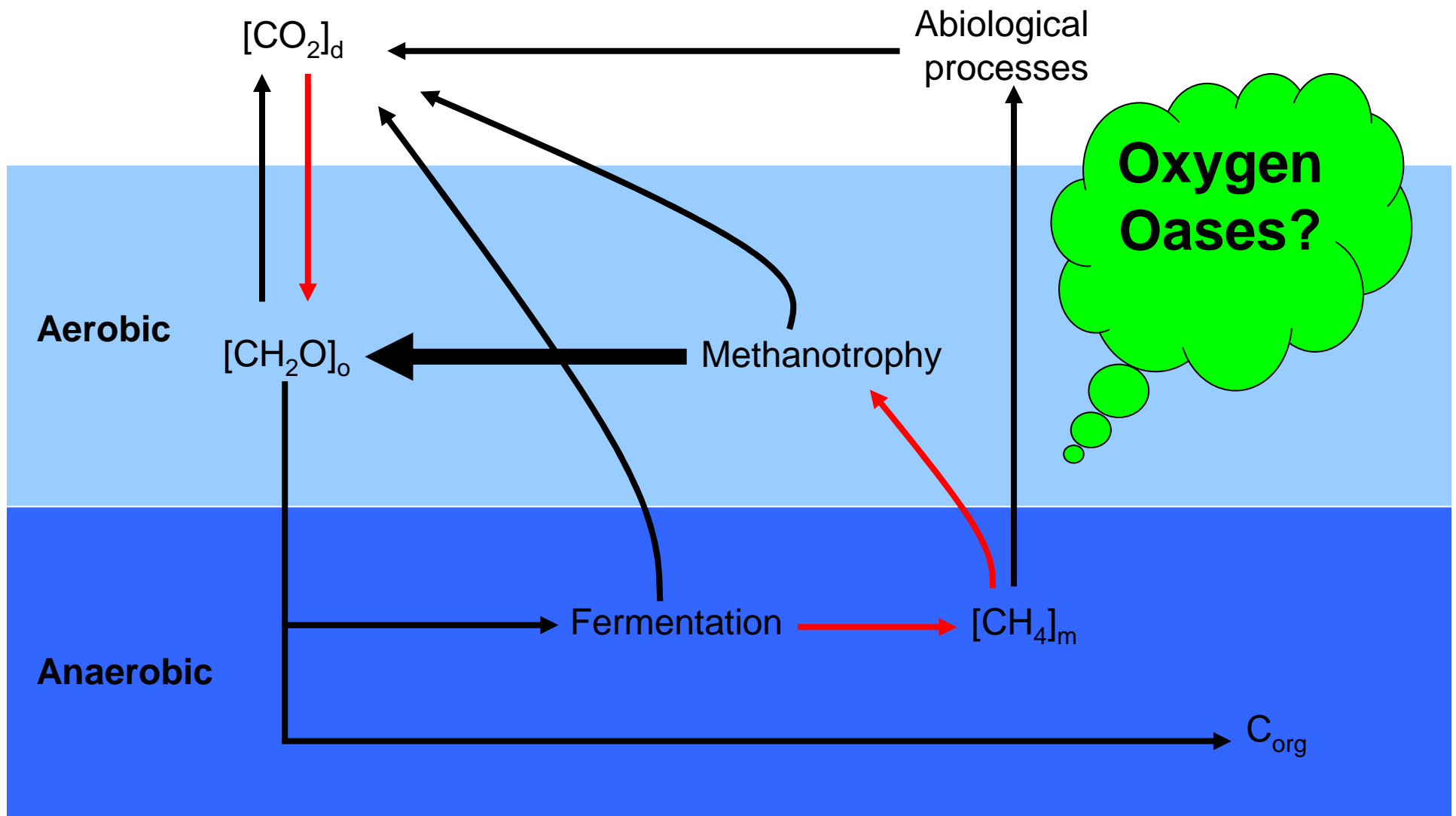
Fractionation effects



Fractionation effects



Fractionation effects

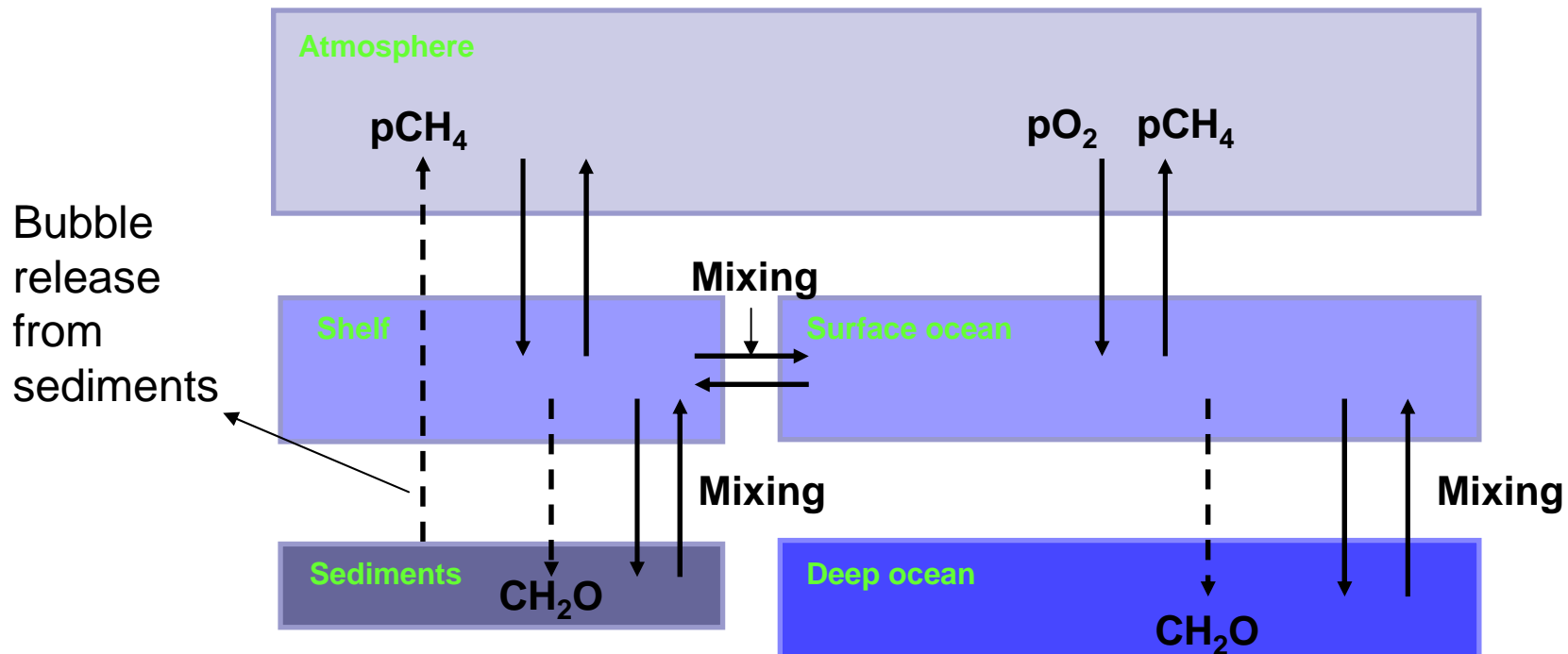




Oxygen oases

- The Hayes Hypothesis: Aerobic methanotrophs may be responsible for the very negative $\delta^{13}\text{C}_{\text{org}}$ signal at *ca* 2.7 Ga, and, consequently, oxygenic photosynthesis “must” have evolved ~300 Ma before the Great Oxidation Event.
- Under what conditions (if any) can the model recreate the observed negative excursion in $\delta^{13}\text{C}_{\text{org}}$?

Model design

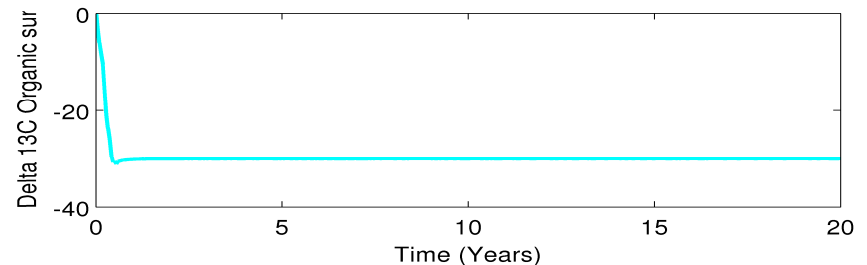
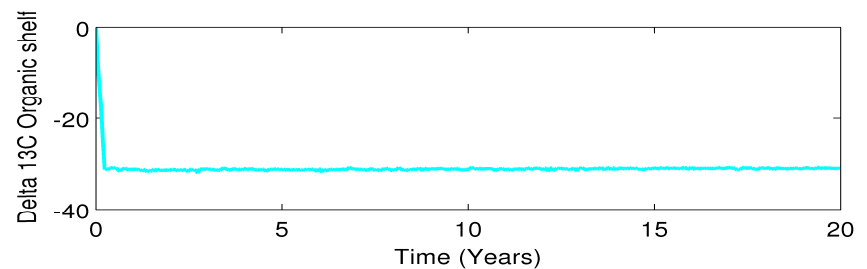


Resources:

Carbon dioxide (CO_2), Water (H_2O)
Oxygen (O_2), Organic carbon (CH_2O)
and Methane (CH_4)

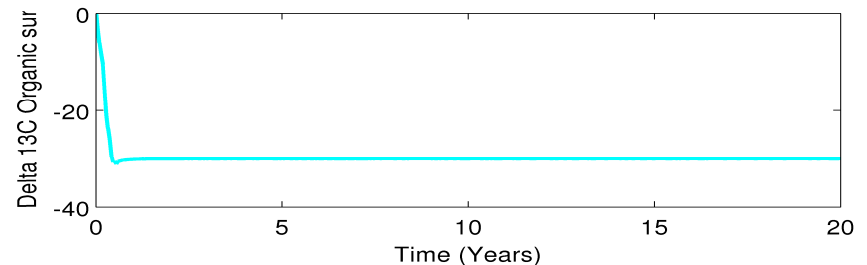
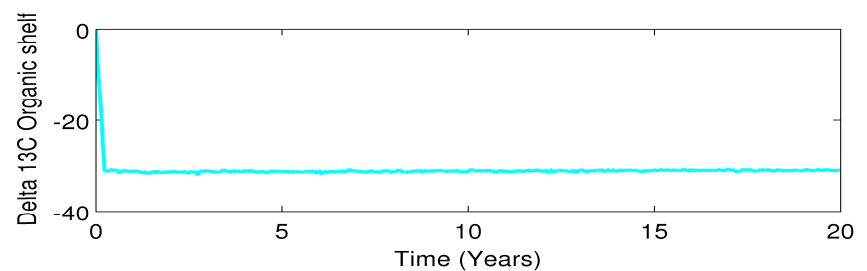
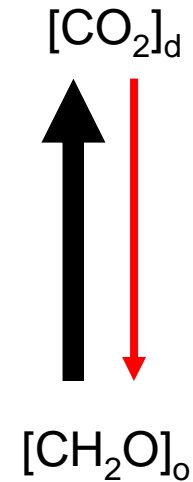
Results – standard run

- The resulting fractionation state of organic carbon in the two surface ocean boxes remains rooted at $\sim -30\text{‰}$.
- The reason for this is that the chemoheterotrophs are dominating the surface ocean populations, meaning little of the organic carbon is channelled through methane.



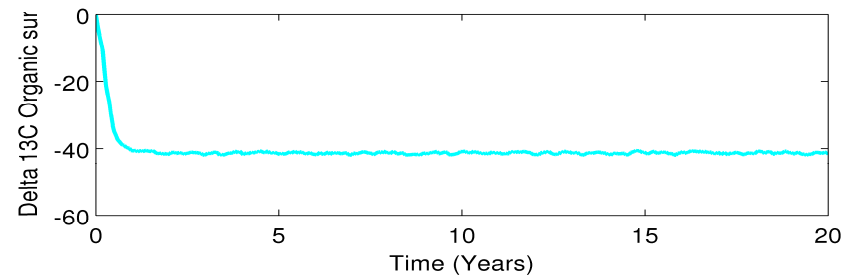
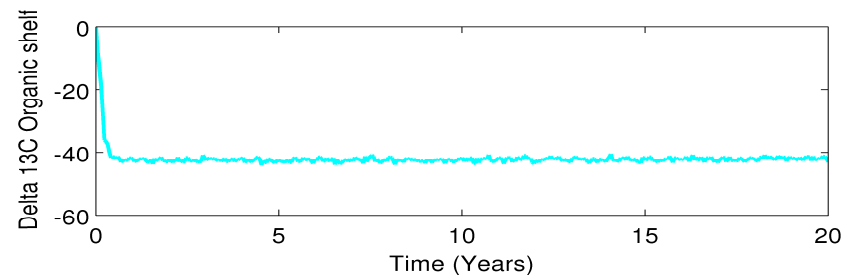
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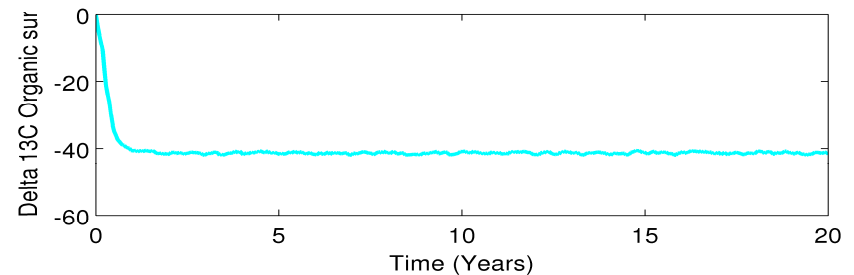
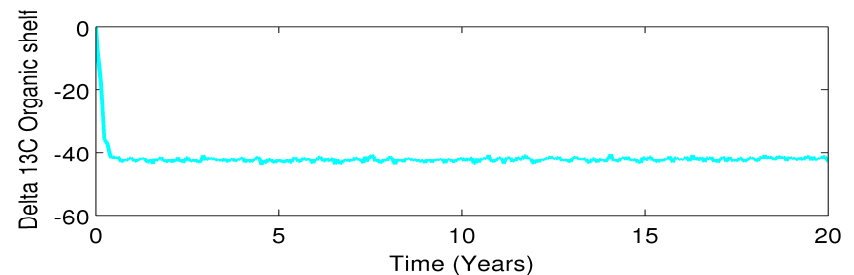
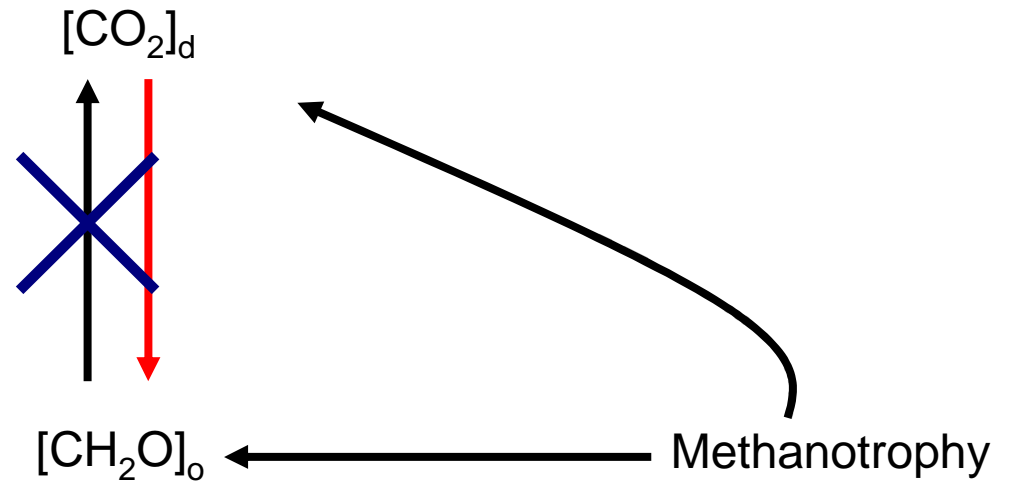
Results - no aerobic chemoheterotrophs

- Despite all of the organic carbon now being channelled through methanogenesis, the resulting fractionation of the organic material only reaches $\sim -40\text{‰}$ in both of the surface locations.
- The conclusion must be that a large part of this methane is being respired, returning the negatively fractionated carbon back to the DIC pool.



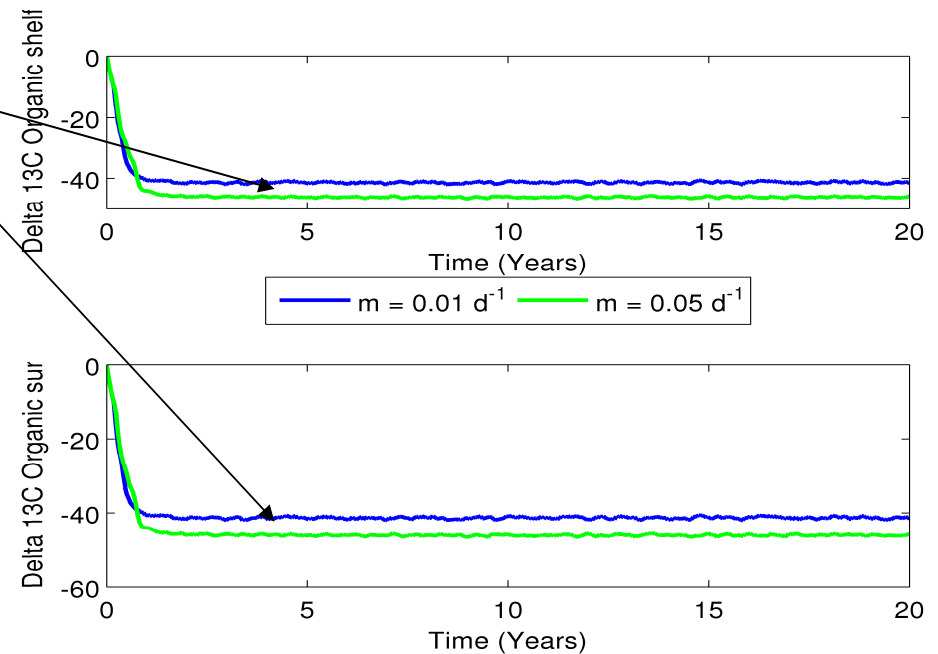
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Results – elevated mortality

- Increasing mortality, which is modelled as a percentage chance that an organism will die at any given time step, goes somewhat towards reducing the signal.
- The effect of this is to increase turn over within the population, meaning more methane is channelled into organic carbon.

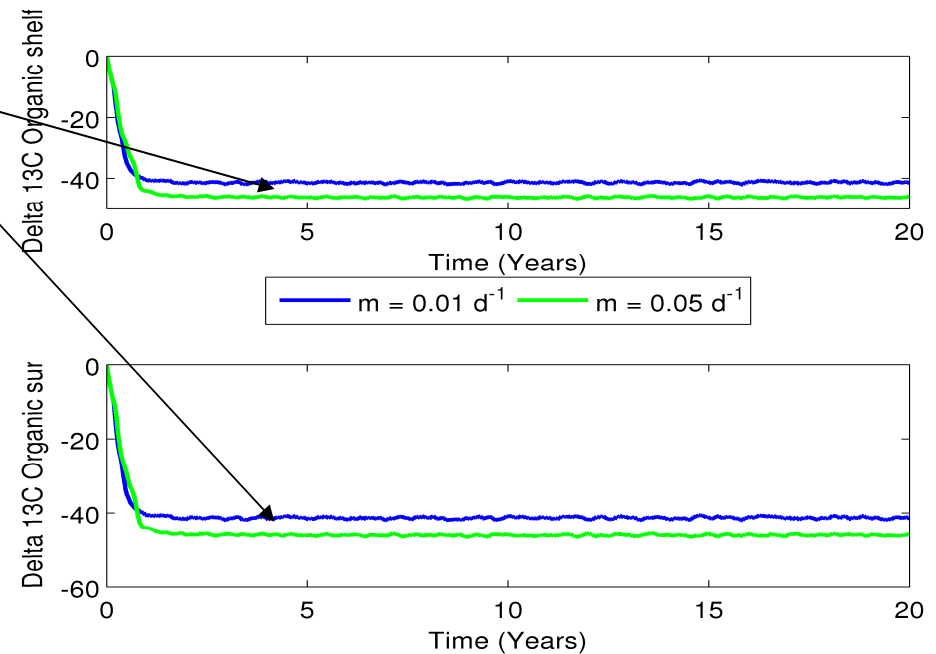


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$[\text{CH}_2\text{O}]_0$ ← Methanotrophy

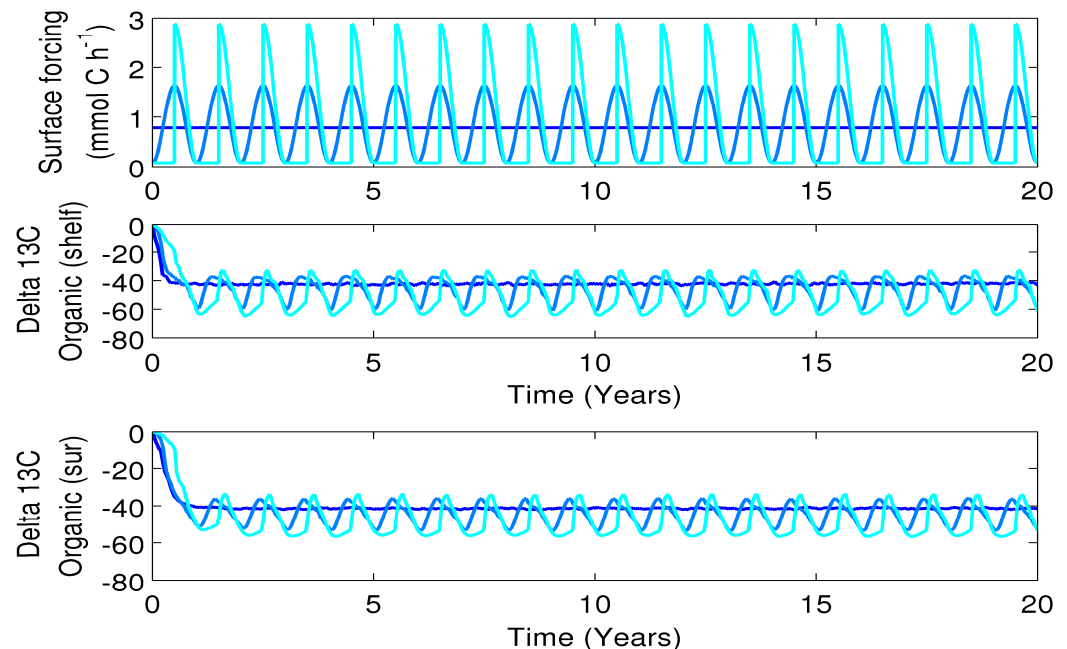
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Results – variable forcing

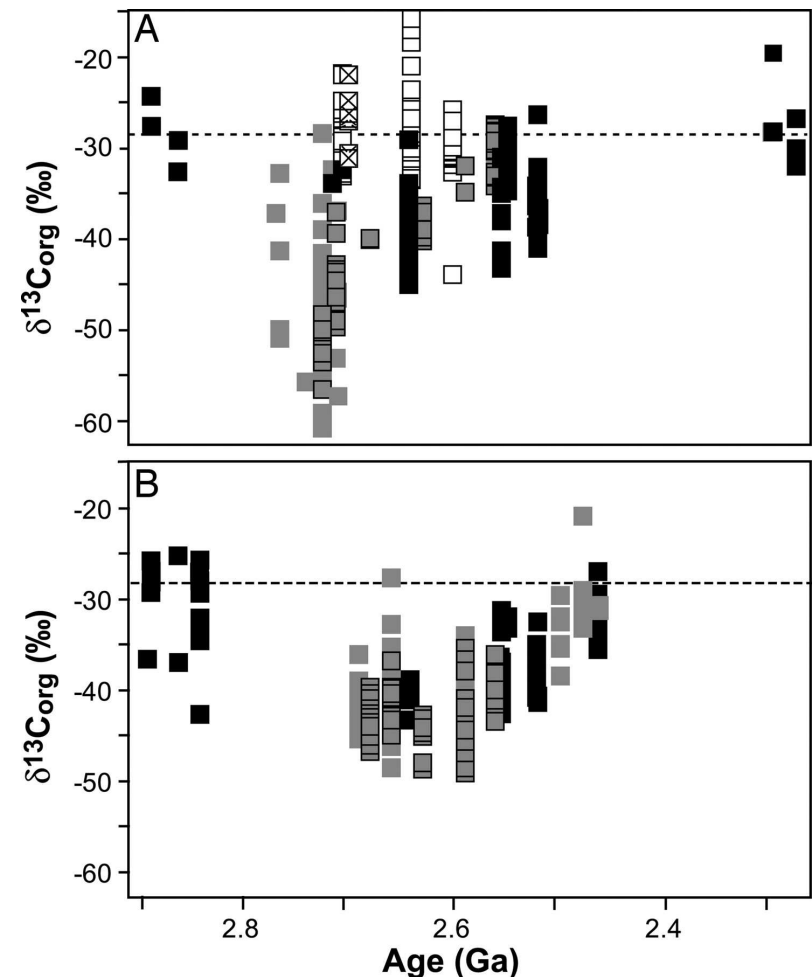
- Very negative fractionation states may be reached, but they require the system to be perturbed.
- By varying productivity within the surface ocean locations, r-strategist populations of methanotrophs tend to emerge.
- These grow fast, channelling large amounts of methane into biomass.

$[\text{CH}_2\text{O}]_0$ ← Methanotrophy



Results

- It is difficult to imagine the very negative signal in $\delta^{13}\text{C}_{\text{org}}$ occurring in the presence of chemoheterotrophs.
- With high levels of mortality, more negative signals emerge.
- In order to achieve a fractionation state $\sim -60\text{‰}$, time varying populations seem to be required.
- This would be consistent with populations of methanotrophs thriving in dynamic coastal or lacustrine environments.





Conclusions

- The agent-based approach explored here makes somewhat tentative progress towards incorporating an adaptive framework into a simple marine ecosystem model through the use of a digital genome.
- Through mutations, and with the inclusion of trade-offs, organisms are able to negotiate trait space, adapting to changing environmental conditions.
- Current/future directions include moving the model into a more modern setting and studying aggregate behaviour:
 - Move from a 0- to 1-D setting (Phil?)
 - Explore more trade-offs in physiological trait values, e.g., quota model (Me)
 - Open up the cell, resource allocation (Stuart?)
- The potential exists for agent-based models to help in the development of population level models by generating emergent aggregate behaviour, that may be later used to train population level representations.