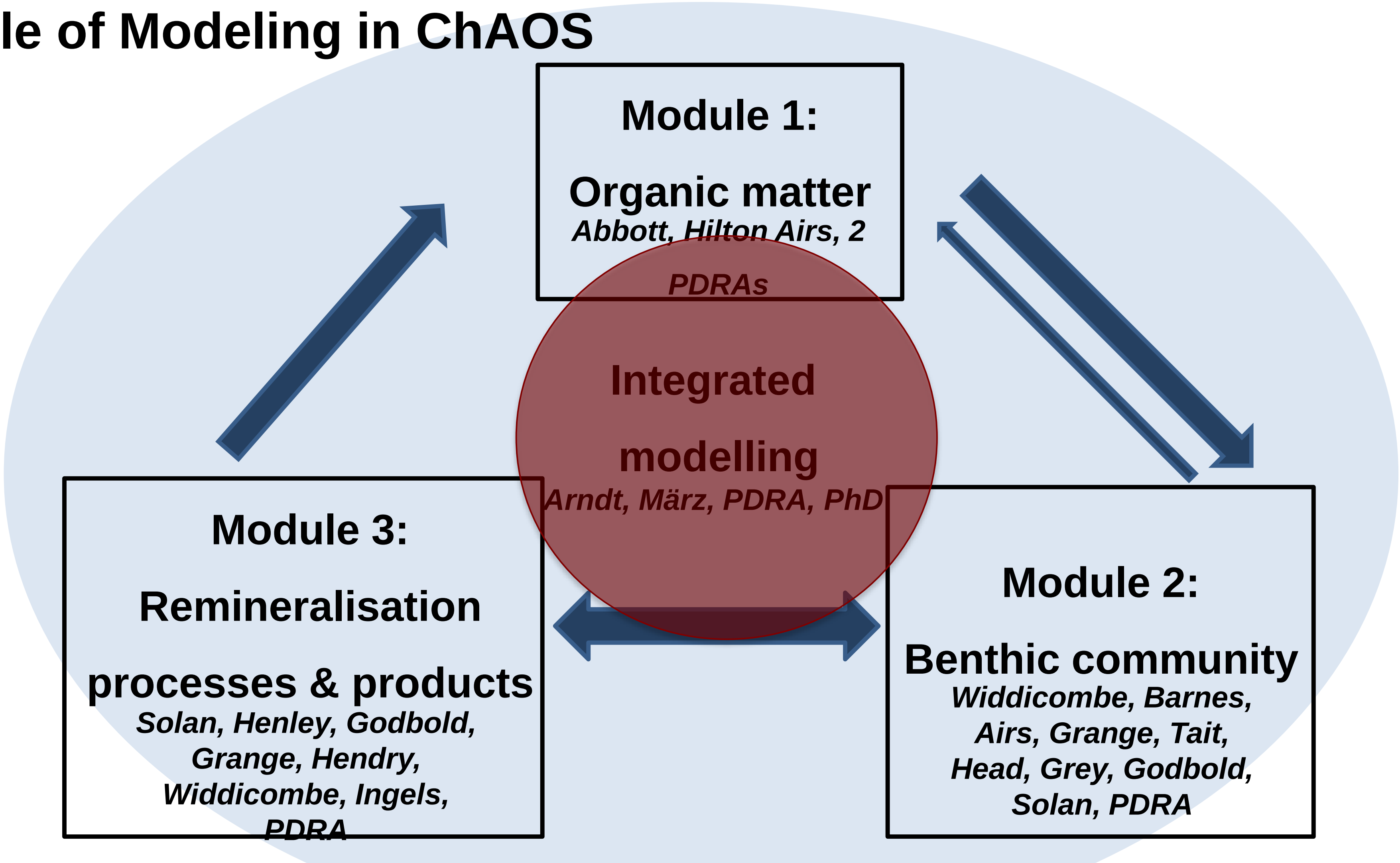
Role of Modeling in ChAOS



Apart from classical roles of quantifying, disentangling, upscaling, predicting, also integrative role.

Modeling provides an important platform for interdisciplinary knowledge synthesis, in which criteria of relevance, the meaning of terms, and the underlying model concepts can be critically discussed

What are we planning to do- more specifically

WP1: Exploring quantitative relationships between OM reactivity its sources and transport pathways and its most important environmental controls, in particular across the studied environmental gradient (**with input from WP2 and 3**)

Deliverable: Generic algorithm for the parameterization of OM degradation models, inform regional predictions

WP2: Explicitly simulate microbial biomass and test the sensitivity of benthic processes on macrofaunal activity

Deliverable: Bioenergetic model that will be used to predict the benthic response to future Arctic climate change

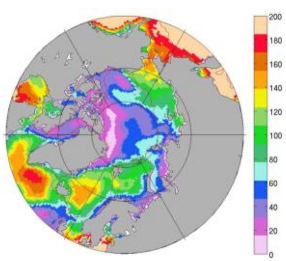
WP3: Quantify benthic process rates and benthic-pelagic exchange fluxes from a local to a regional scale and explore transient dynamics (e.g. on seasonal and climate change relevant scales)

Deliverable: Local -> regional quantification of benthic process rates and exchange fluxes (1980-299)

Methods

Local Scale/ Transient Simulations (PGRA, PDRA)

Reaction-transport models (RTMs), with explicit biomass description



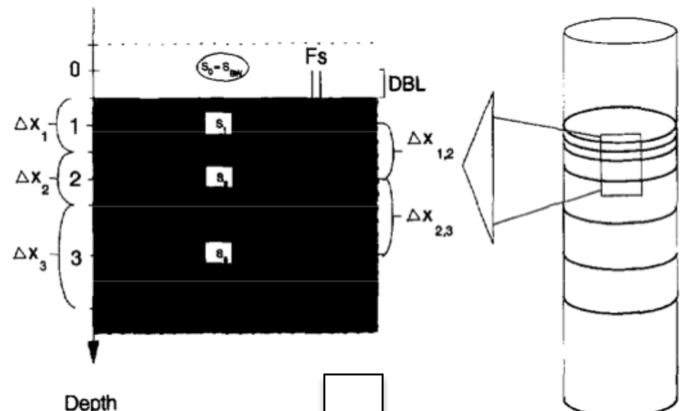
Regional Scale/ Longterm Predictions (PDRA)

Numerically efficient encapsulation of RTM forced by **regional model (e.g. NEMO-MEDUSA; PISCES)** results

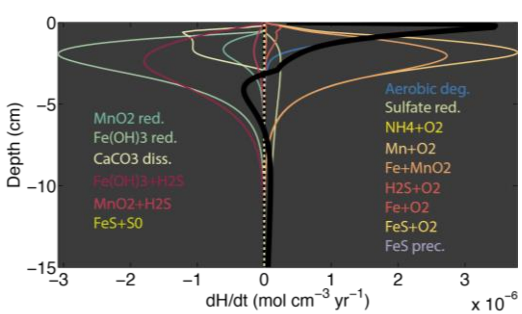
The Art of Reaction-Transport Modeling: General Approach

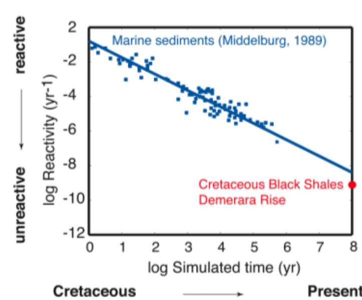
INPUT: Depth-Profiles, Bottom-water conditions, sedimentation rate, porosity, macrobenthic activity for model parameterization, forcing, calibration/validation

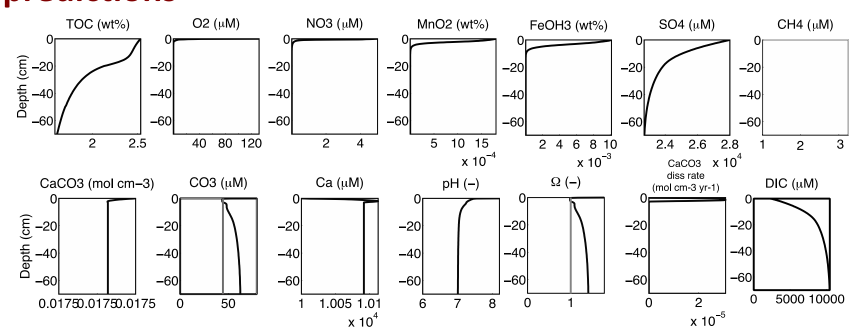
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(vC + D\frac{\partial C}{\partial x}\right) + \sum_i R_i$$



OUTPUT: Rates, benthic recycling and burial fluxes, budgets, rate constants
-> inform transient simulations, regional upscaling and future predictions

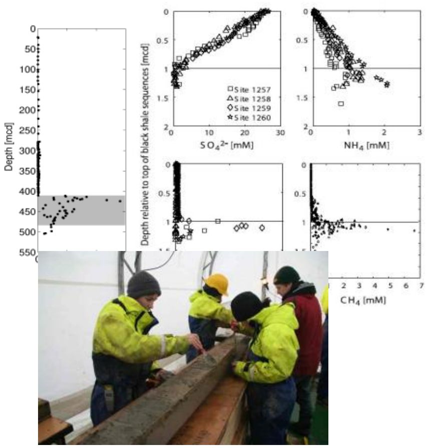






The Art of Reaction-Transport Modelling: Process

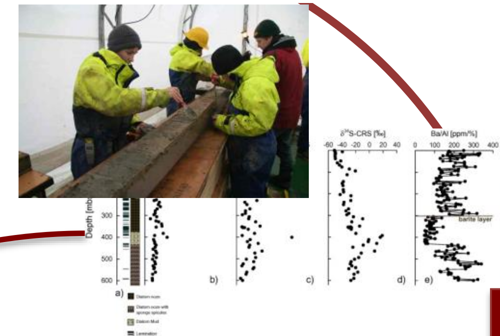
1 Formulate Hypothesis/ Question



2 Design Reaction-Transport Model

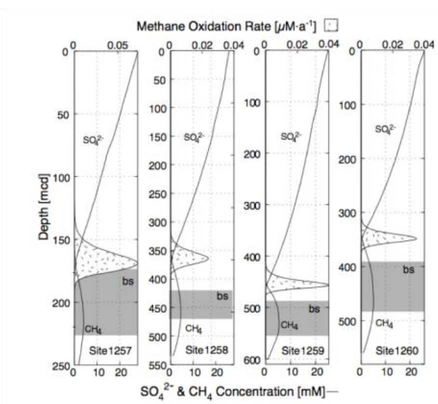
$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(vC + D\frac{\partial C}{\partial x}\right) + \sum_i R_i$$

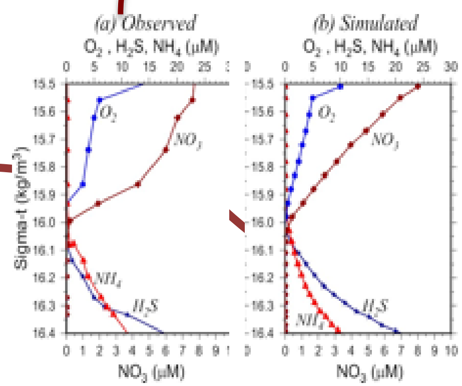
3 Constrain parameters, forcings,..



4 Run model forward

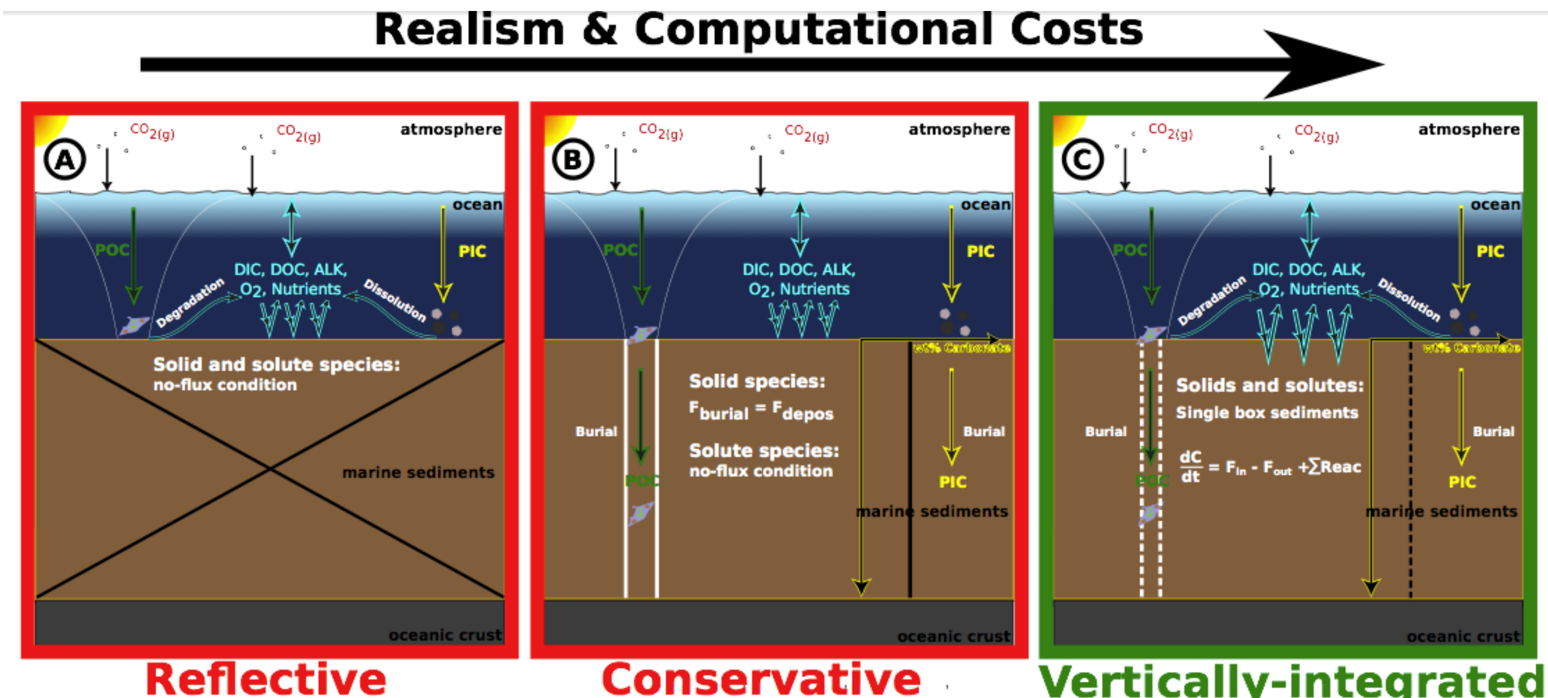
5 Compare model results and observations

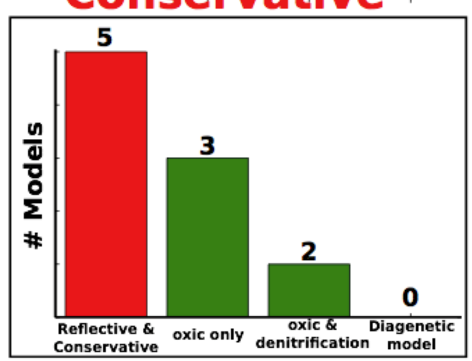




The Art of Reaction-Transport Modelling: Upscaling

Problem: vertically resolved, multi-component diagenetic models are computationally expensive -> direct coupling to regional/global models not possible



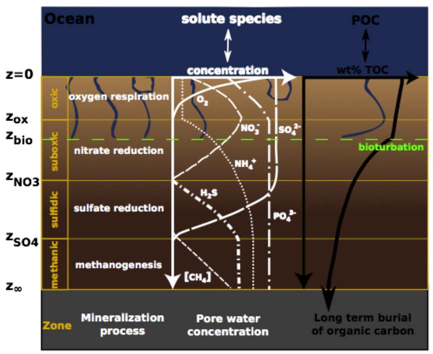


Hülse et al. , Earth-Sci. Rev., in review

The Art of Reaction-Transport Modelling: Upscaling

Solution: Numerically efficient approach

Analytical Solution of 1D RT Equations:
e.g. OMEN-SED (Huelse & Arndt)



Hülse et al., GMD, in prep.

Vertically resolved, steady-state advection-diffusion-reaction equation:

$$\frac{\partial C_i}{\partial t} = 0 = D\frac{\partial^2 C_i}{\partial z^2} - w\frac{\partial C_i}{\partial z} - \sum_i \alpha_i \exp(-\beta_i z) - k \cdot C + Q$$

The ODE solution is of the general form:

$$C(z) = A\exp(az) + B\exp(bz) + \sum_i \frac{\alpha_i}{D\beta_i^2 - w\beta_i - k} \cdot \exp(-\beta_i z) + \frac{Q}{k}$$

D: Diffusion coefficient
w: Advection/burial rate

Primary redox reactions	Degradation of organic matter via aerobic respiration, denitrification, sulfate reduction, methanogenesis (implicit)
Secondary redox reactions	Oxidation of ammonium and sulfide by oxygen, anaerobic oxidation of methane by sulfate
Adsorption/Desorption	Ad-/Desorption of P on/from $Fe(OH)_3$, NH_4 adsorption, PO_4 adsorption
Mineral precipitation	Formation of authigenic P
Variables	Organic matter, oxygen, nitrate, ammonium, sulfate, sulfide (hydrogen sulfide), phosphate, Fe-bound P, DIC, ALK

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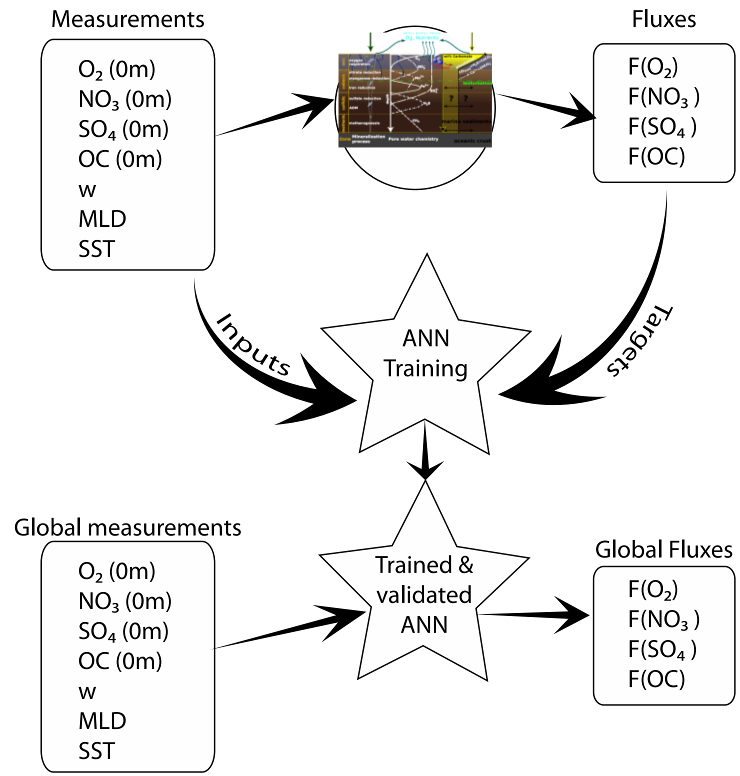
Artificial Neural Network:
(Pika & Arndt)

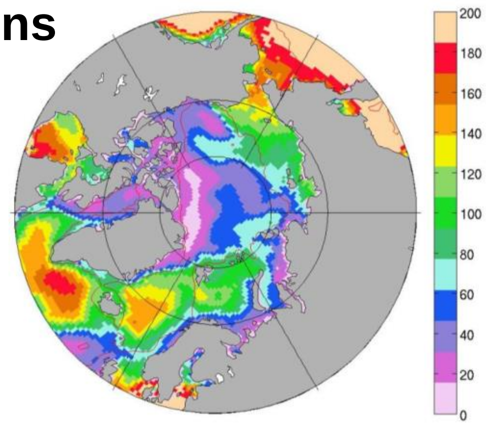


The Art of Reaction-Transport Modelling: Upscaling

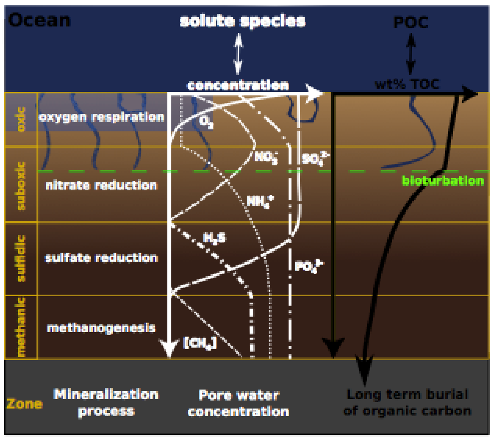
Coupling to regional model (e.g. MEDUSA)/ or stand-alone forced by regional observations

Bottom water concentrations
TOC, O_2, NO_3, SO_4, NH_4, H_2S, PO_4…

NEMO-MEDUSA (online/offline) or observations



OMEN-SED/ANN

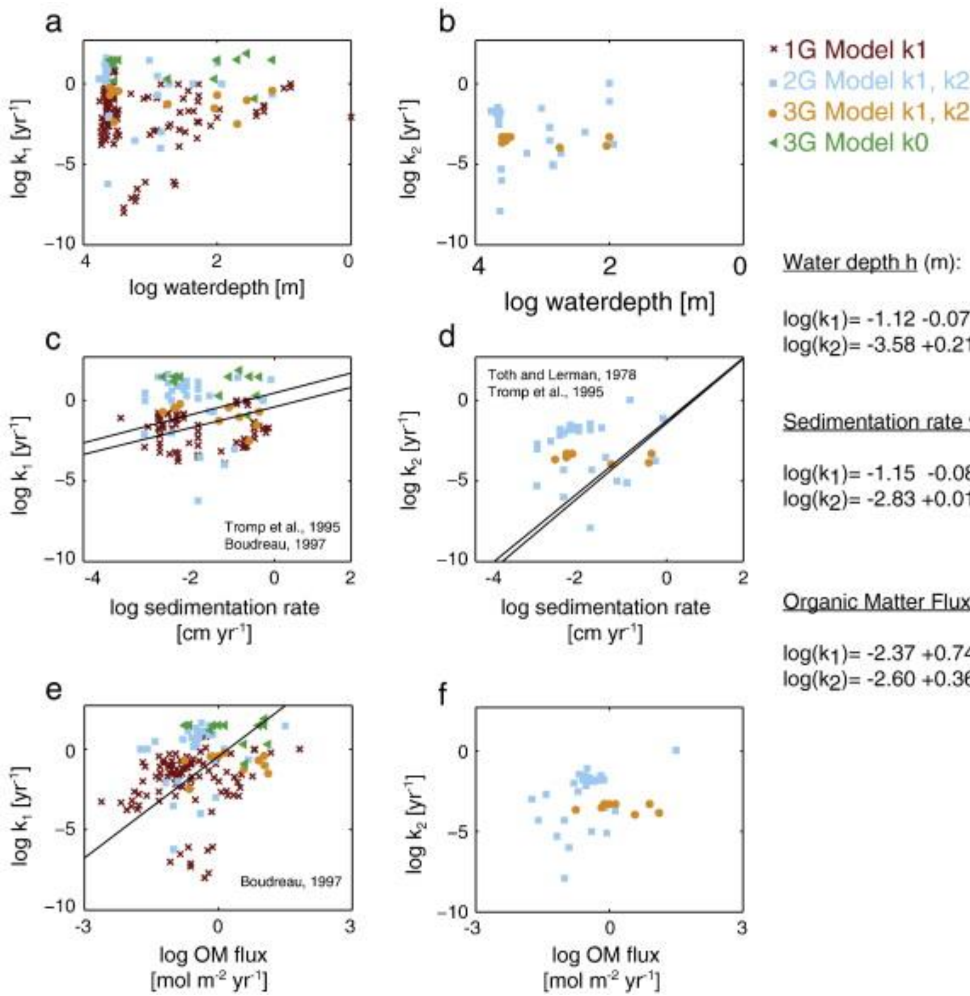


TOC burial,
SWI fluxes O2, NO3, SO4, NH4, H2S, PO4…

Specific Model objectives

WP1: Exploring quantitative relationships between OM reactivity its sources and transport pathways and its most important environmental controls, in particular across the studied environmental gradient

Rational: No mechanistic framework to quantify OM degradation rate constants (reactivity) in data-poor areas -> huge challenge for regional/global biogeochemical models



Water depth h (m):

$\log(k_1) = -1.12 - 0.077 \cdot \log(h)$ $R^2=0.001$
$\log(k_2) = -3.58 + 0.218 \cdot \log(h)$ $R^2=0.007$

Sedimentation rate w (cm yr^{-1}):

$\log(k_1) = -1.15 - 0.080 \cdot \log(w)$ $R^2=0.0024$
$\log(k_2) = -2.83 + 0.013 \cdot \log(w)$ $R^2=5e-05$

Organic Matter Flux F_G (mol m^{-2} yr^{-1}):

$\log(k_1) = -2.37 + 0.740 \cdot \log(F_G)$ $R^2=0.08$
$\log(k_2) = -2.60 + 0.363 \cdot \log(F_G)$ $R^2=0.03$

Specific Model objectives

WP1: Exploring quantitative relationships between OM reactivity its sources and transport pathways and its most important environmental controls, in particular across the studied environmental gradient (**with input from WP2 and 3**)

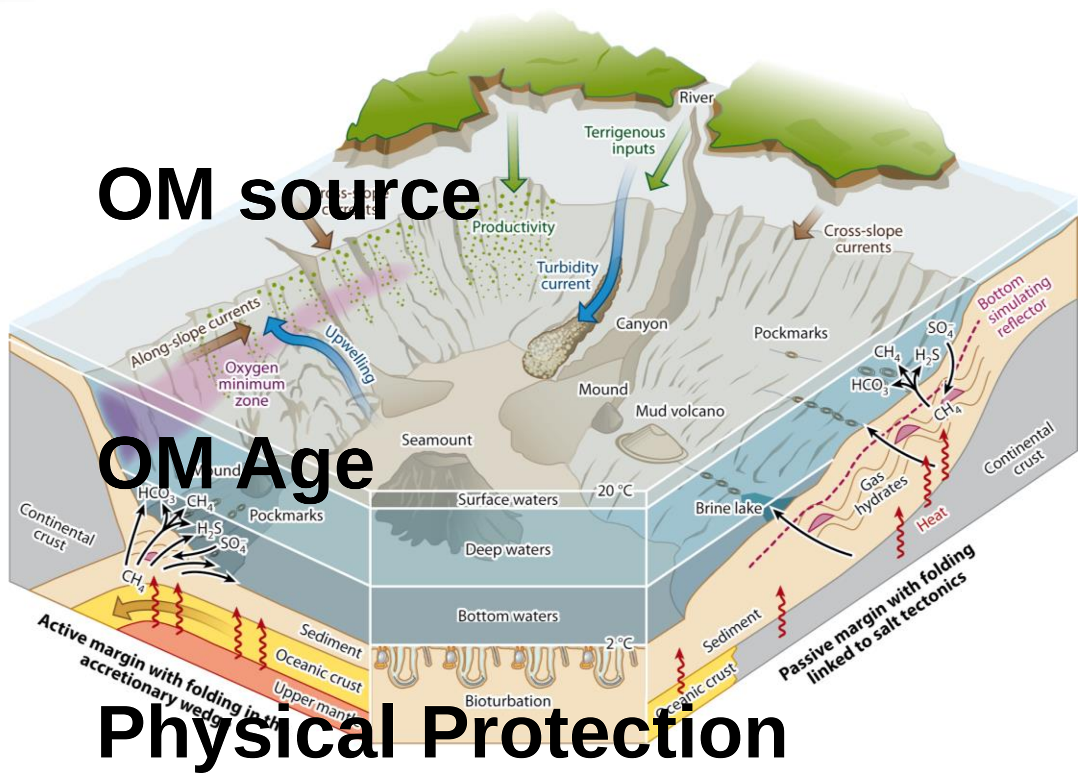
Idea: explore links between apparent reactivity, determined by diagentic modeling with environmental controls

k = f

OM source

OM Age

Physical Protection

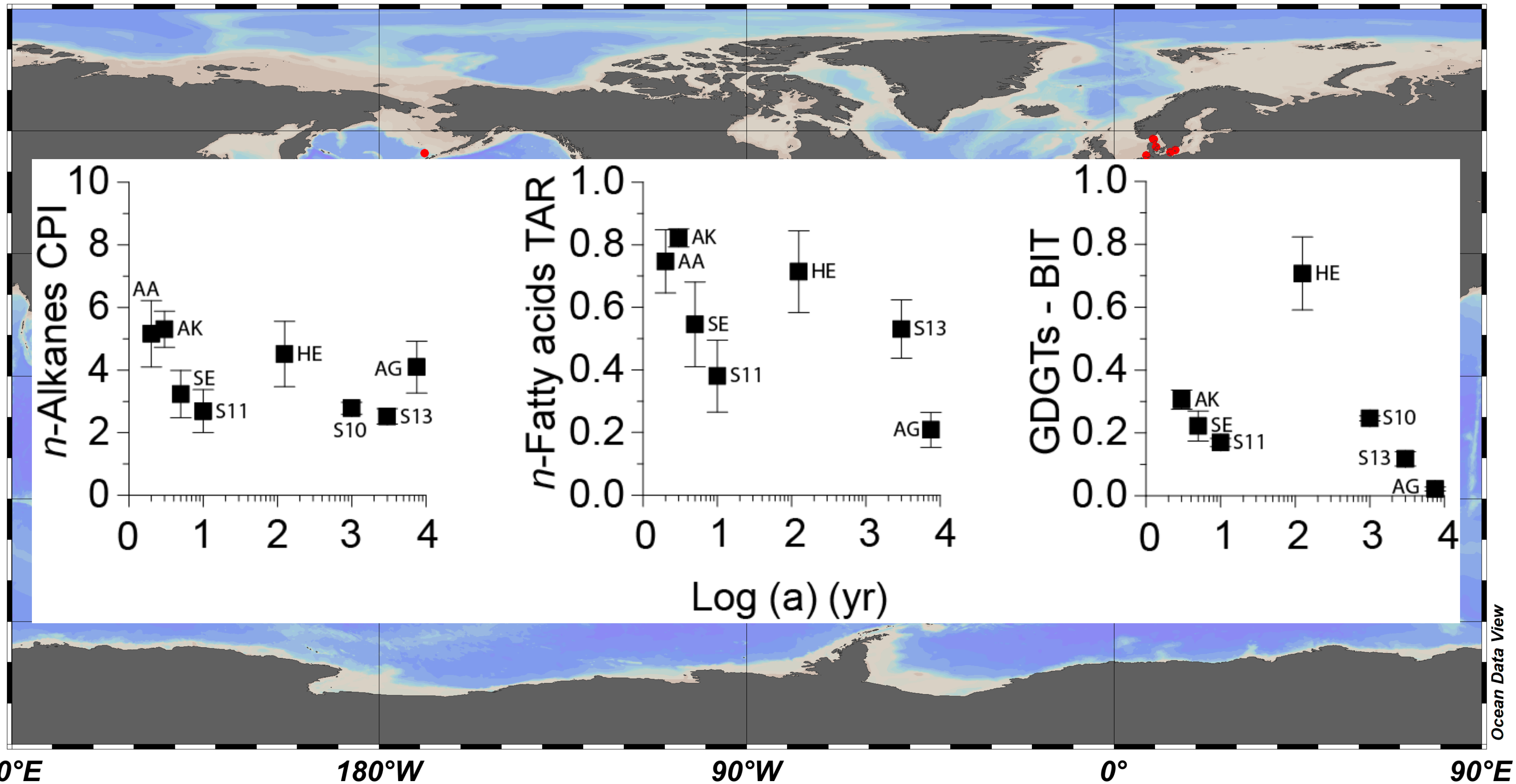


Levin LA, Sibuet M. 2012.
Annu. Rev. Mar. Sci. 4:79–112

Specific Model objectives

WP1: Exploring quantitative relationships between OM reactivity its sources and transport pathways and its most important environmental controls, in particular across the studied environmental gradient

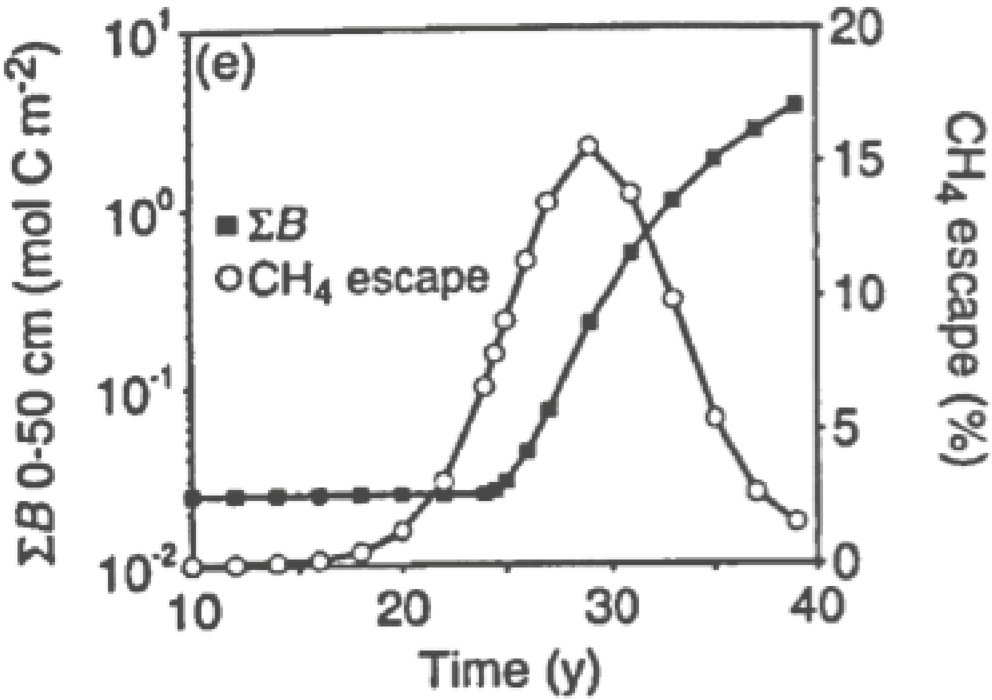
Complementary ongoing work (Salles de Freitas, Arndt, Pancost): explore link between lipid biomarkers and organic matter degradation rate constants (extracted by diagenetic modelling) across different environments



Specific Model objectives

WP2: Explicitly simulate microbial biomass and test the sensitivity of benthic processes on macrofaunal activity

Rational: Microbial biomass is generally not explicitly resolved in diagentic models, but plays an important role in determining the transient response to changing conditions

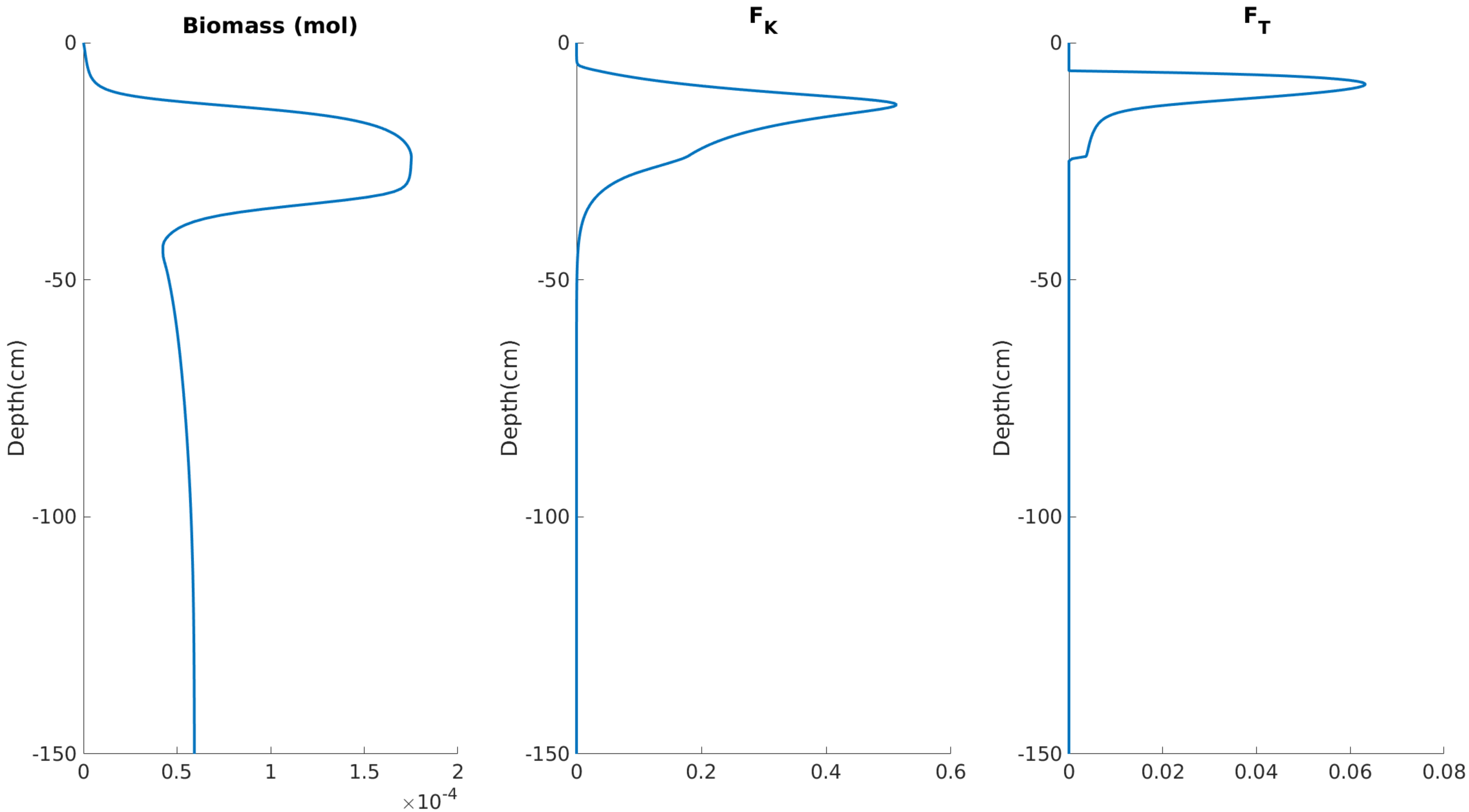


Dale et al., 2009

Specific Model objectives

WP2: Explicitly simulate microbial biomass and test the sensitivity of benthic processes on macrofaunal activity

Idea: Develop bioenergetic model to account for kinetic and thermodynamic controls- e.g. bioenergetic response to methane flux (Puglini & Arndt)



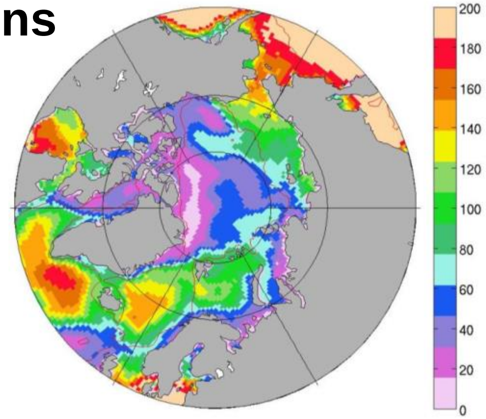
Specific Model objectives

WP3: Quantify benthic process rates and benthic-pelagic exchange fluxes from a local to a regional scale and explore transient dynamics (e.g. on seasonal and climate change relevant scales)

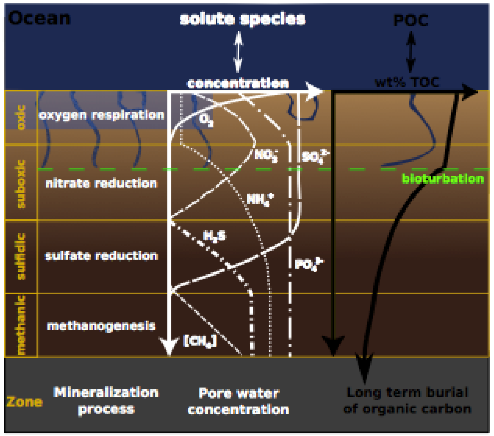
Rational: No regional scale estimates, no predictions of benthic response to future change due to lack of upscaling approaches

Bottom water concentrations
TOC, O_2, NO_3, SO_4, NH_4, H_2S, PO_4...

NEMO-MEDUSA (online/offline) or observations



OMEN-SED/ANN



TOC burial,
SWI fluxes O2, NO3, SO4, NH4, H2S, PO4...

Specific Model objectives

WP3: Quantify benthic process rates and benthic-pelagic exchange fluxes from a local to a regional scale and explore transient dynamics (e.g. on seasonal and climate change relevant scales)

Idea: Use numerically efficient encapsulations of the diagenetic model forced with Earth System model output to calculate regional fluxes and predict future change
Complementary ongoing work: (Huelse & Arndt) OMEN-SED + cGENIE (Earth System Model of Intermediate Complexity) simulation of benthic-pelagic exchange fluxes at a global scale