Using R to Model Complex Biogeochemical Systems

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Introduction to the science
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  - 71% of Earth’s surface (335,258,000 km²)
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  - Globally important sinks & sources for nutrients
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  - High rates of primary productivity
The maths…
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- Change in concentration of i
- Transport of chemical species
- Rate of consumption of i, but dependent on j
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R_{O_2} = \kappa[OM] \left( \frac{[O_2]}{[O_2] + k_{s_{oxic}}} \right)
\]
Transport
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  ```r
  Grid <- setup.grid.1D(N=100, dx.1=0.1, L=15)
  - Grid$x.mid, Grid$x.int, Grid$dx
  
  O2tran <- tran.1D (C=O2, C.up=bwO2, dx=Grid)
  - Other arguments allow specific transport terms to be used
  ```
Solving the maths
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  - rootSolve: ‘Nonlinear root finding, equilibrium and steady-state analysis of ordinary differential equations’
  - deSolve: ‘General solvers for initial value problems of ordinary differential equations (ODE), partial differential equations (PDE), differential algebraic equations (DAE), and delay differential equations (DDE).’
Solving the maths (cont...)
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– Simple to implement
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```r
modelFunction <- function(t, y, pars){
  # implementation of transport and differential equations; e.g:
  OC <- y[1:100]; O2 <- y[101:200]
  oxicMin <- r*OC*(O2/(O2+ksO2oxic))
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dyn.output <- ode.1D(y=ss.output$y, times=0:364,
    func=modelFunction, parms=pars)
Data management

- Data
  - Multiple sites, cruises, repeat measurements & parameters
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- Multiple sites, cruises, repeat measurements

- Parameters

- North Dogger
- Tyne
- Osyter Grounds
- Sean Gasfields
- Warp

OMC - Martin Weinelt
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- Allows model calibration to be carried out
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  - Allows us to discover the most sensitive model parameters
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  - Greater access for non-modeller researchers
  - Public engagement of science
Any questions?

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