Building an Open Source work bench for marine biogeochemical models of the water column

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- Why an ecosystem model work bench ?
- GOTM - A physical water column model
  - Turbulence models in GOTM
  - GOTM examples
- Positivity and conservation
- Coupling GOTM with BIO: Current status
- GOTM-BIO example
- Road Map

Motivation

Biogeochemical models strongly depend on the physical model into which they are embedded.

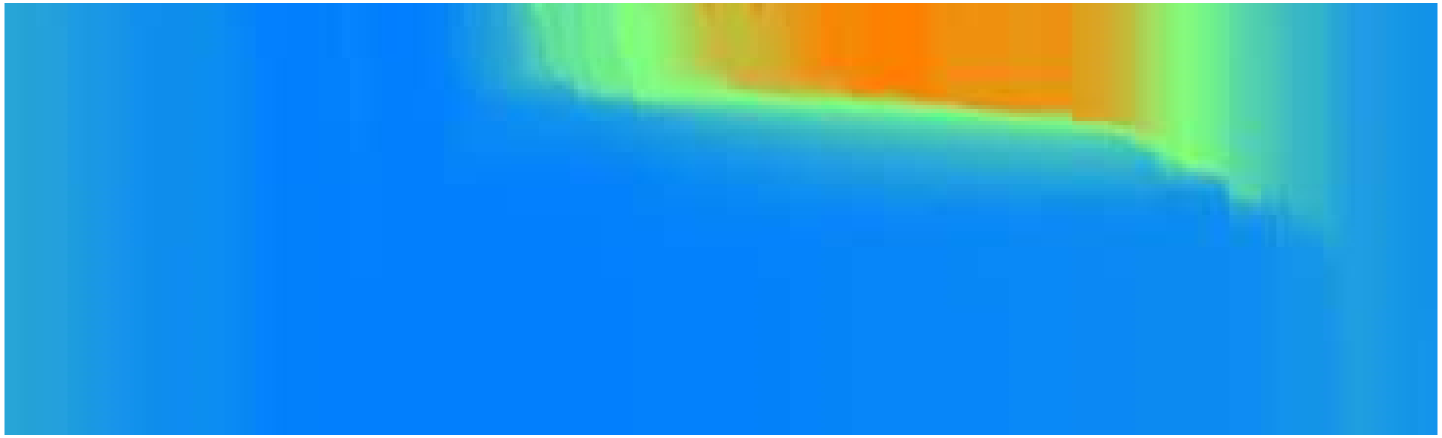
$\Rightarrow$ They can only be compared to each others in identical physical frames.

$\Rightarrow$ GOTM-BIO may be such a framework.

Motivation

Northern North Sea temperature

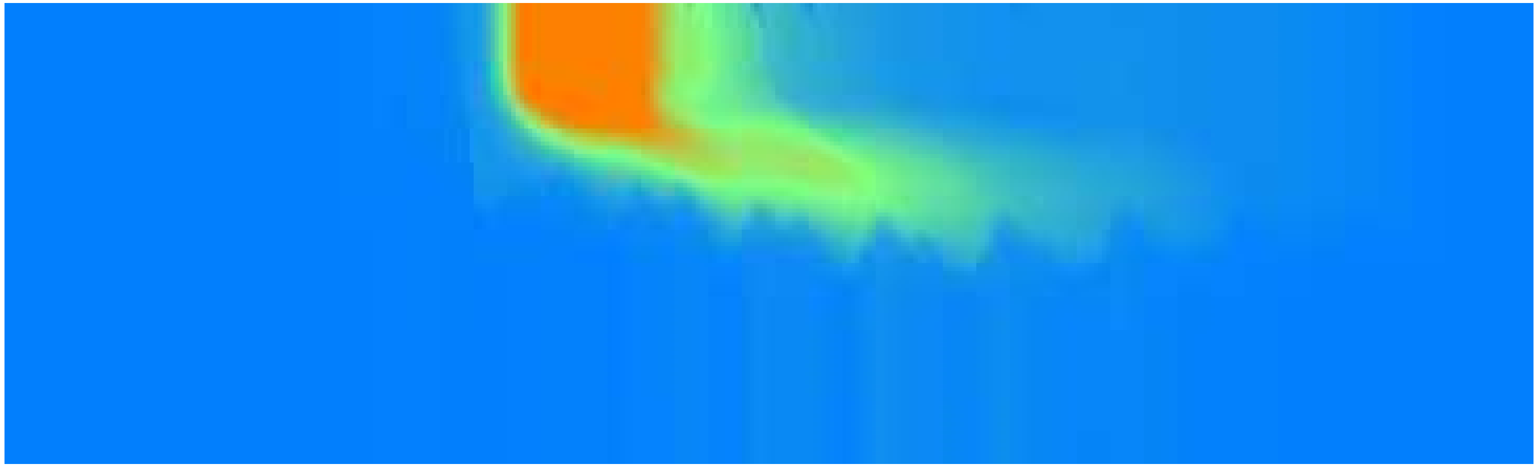
- simulation with GOTM
- annual run for 1998
- 110 m water depth
- realistic forcing



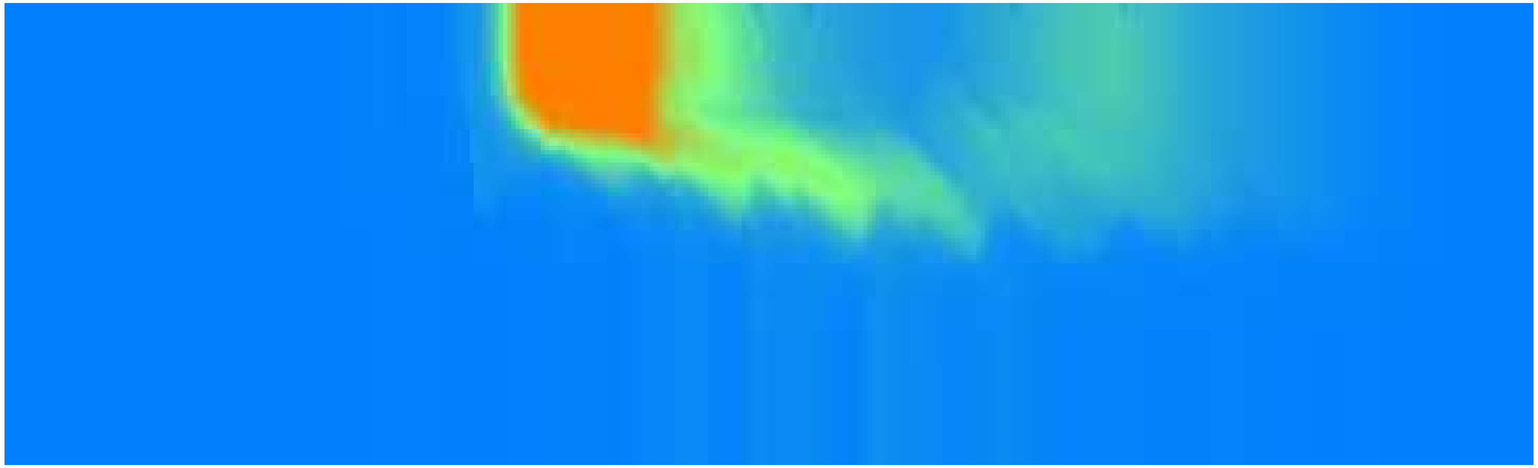
Range: $7^\circ C$ – $14^\circ C$

Motivation

Phytoplankton (NPZD-model, internal wave mixing):



Phytoplankton (NPZD-model, no internal wave mixing):



GOTM, http://www.gotm.net

General Ocean Turbulence Model

Challenge
- Aim
- The Idea
- Key features

Software
- Fortran code
- Test cases
- Forcing
- How to run?

Information
- What's New
- Publications
- E-mail list
- FAQ
- User Group
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GOTM is a one-dimensional numerical model developed and supported by a core team of ocean modellers. GOTM aims at simulating accurately vertical exchange processes in the marine environment where mixing is known to play a key role. GOTM is freely available under the GPL (Gnu Public License).

The interested user can download the source code, a set of test cases (Papa, November, Flex, ...) and a comprehensive report.

You are warmly invited to join the GOTM mailing list and send any comments/questions to the GOTM team or become a GOTM contributor. The GOTM developers are grateful to their sponsors.

Page "www.gotm.net" maintained by webmaster. Last update: 10/28/00 18:10:02

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GOTM: Algebraic SMCs

Turbulent Fluxes:

$$\langle \tilde{u}\tilde{w} \rangle = -\nu_t \partial_z \bar{u}, \quad \langle \tilde{w}\tilde{T} \rangle = -\nu_t' \partial_z \bar{T}$$

Eddy Viscosity / Eddy Diffusivity:

$$\nu_t = c_\mu(\alpha_M, \alpha_N)\frac{k^2}{\varepsilon}, \quad \nu_t' = c_\mu'(\alpha_M, \alpha_N)\frac{k^2}{\varepsilon}.$$

Shear Number, Buoyancy Number:

$$\alpha_M = \frac{k^2}{\varepsilon^2}M^2, \quad \alpha_N = \frac{k^2}{\varepsilon^2}N^2.$$

GOTM: TKE-Equation

$$\partial_t k - \partial_z \left(\frac{\nu_t}{\sigma_k} \partial_z k \right) = P + B - \varepsilon,$$

$$L \propto \frac{k^{3/2}}{\varepsilon} \qquad (1)$$

k	turbulent kinetic energy
P	shear production
B	buoyancy production
ε	viscous dissipation
L	macro length scale

GOTM: Length scale equations

k-ε model (*Launder and Spalding* [1972]):

$$\partial_t \varepsilon - \partial_z \left(\frac{\nu_t}{\sigma_\varepsilon} \partial_z \varepsilon \right) = \frac{\varepsilon}{k} \left(c_{\varepsilon 1} P + c_{\varepsilon 3} B - c_{\varepsilon 2} \varepsilon \right) .$$

k-kL model (*Mellor and Yamada* [1982]):

$$\partial_t \left(kL \right) - \partial_z \left(S_l \partial_z (kL) \right) =$$

$$\frac{L}{2} \left[E_1 P + E_3 B - \left(1 + E_2 \left(\frac{L}{L_z} \right)^2 \right) \varepsilon \right] .$$

GOTM: Length scale equations

k-ω model (*Wilcox* [1988], *Umlauf et al.* [2003]):

$$\partial_t \omega - \partial_z \left(\frac{\nu_t}{\sigma_\omega} \partial_z \omega \right) = \frac{\omega}{k} \left(c_{\omega 1} P + c_{\omega 3} B - c_{\omega 2} \varepsilon \right) , \quad \omega = \frac{\varepsilon}{k} .$$

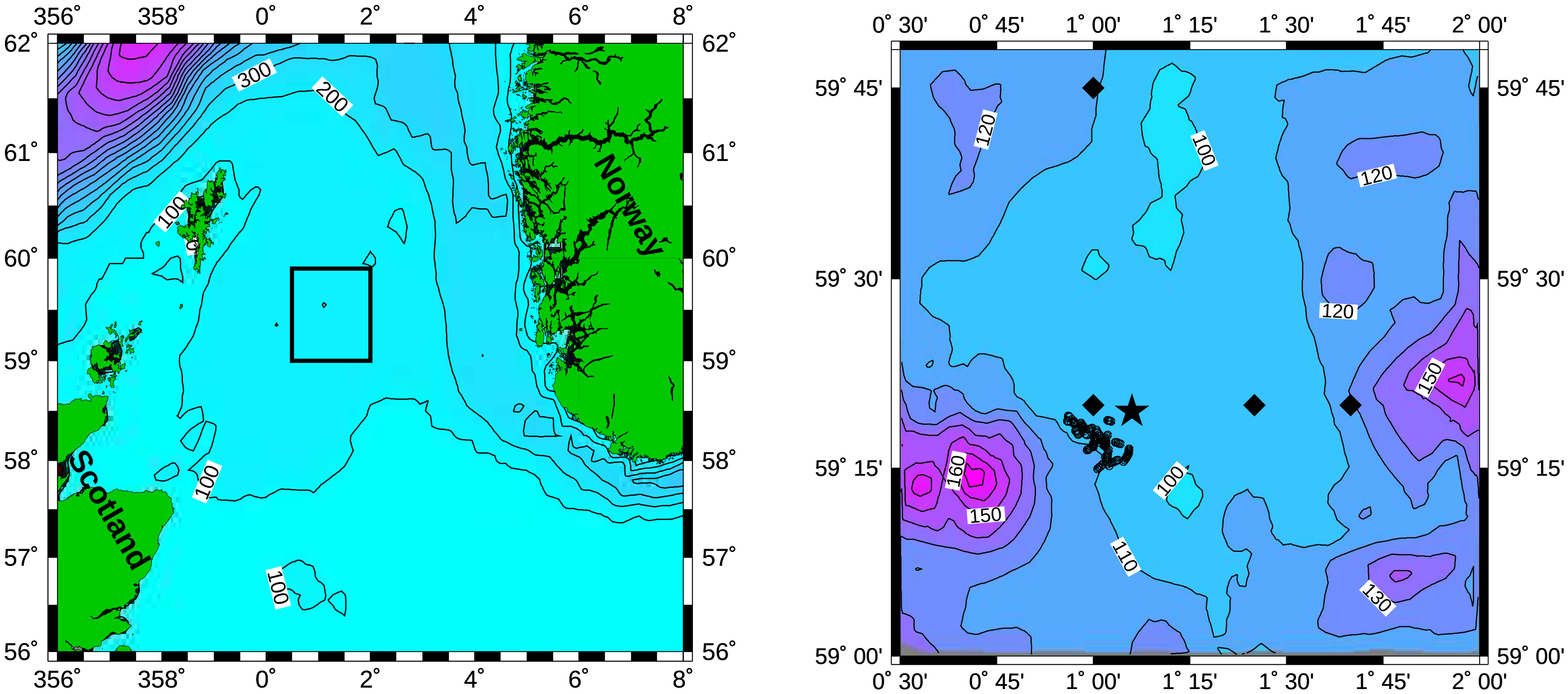
Generic model (*Umlauf and Burchard* [2003]):

$$\partial_t \left(k^m L^n \right) - \partial_z \left(\frac{\nu_t}{\sigma_{mn}} \partial_z \left(k^m L^n \right) \right) =$$

$$k^{m-1} L^n \left(c_{nm1} P + c_{mn3} B - c_{mn2} \varepsilon \right) .$$

GOTM: Northern North Sea

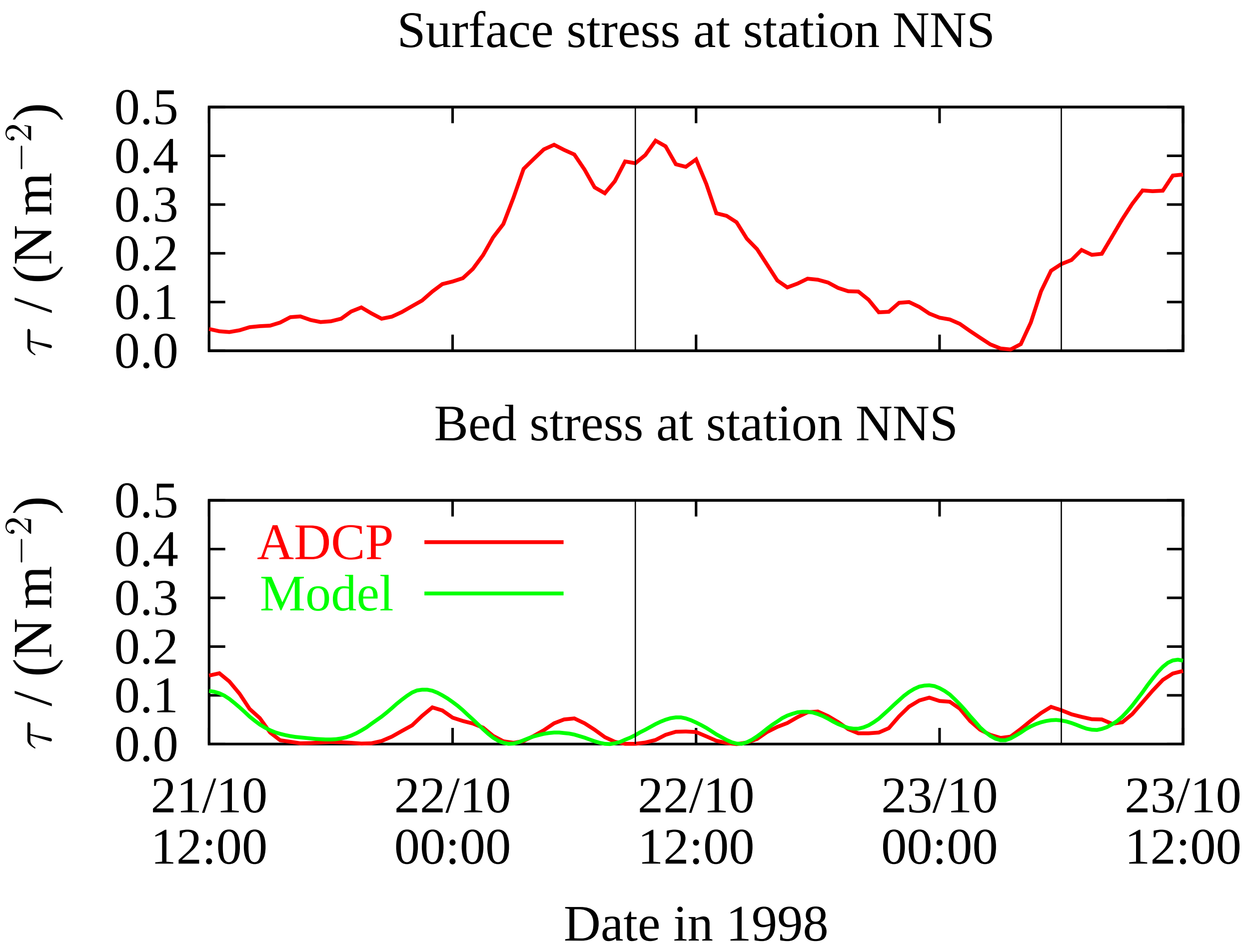
Bathymetry and station map



Burchard et al. [2002]

GOTM: Northern North Sea

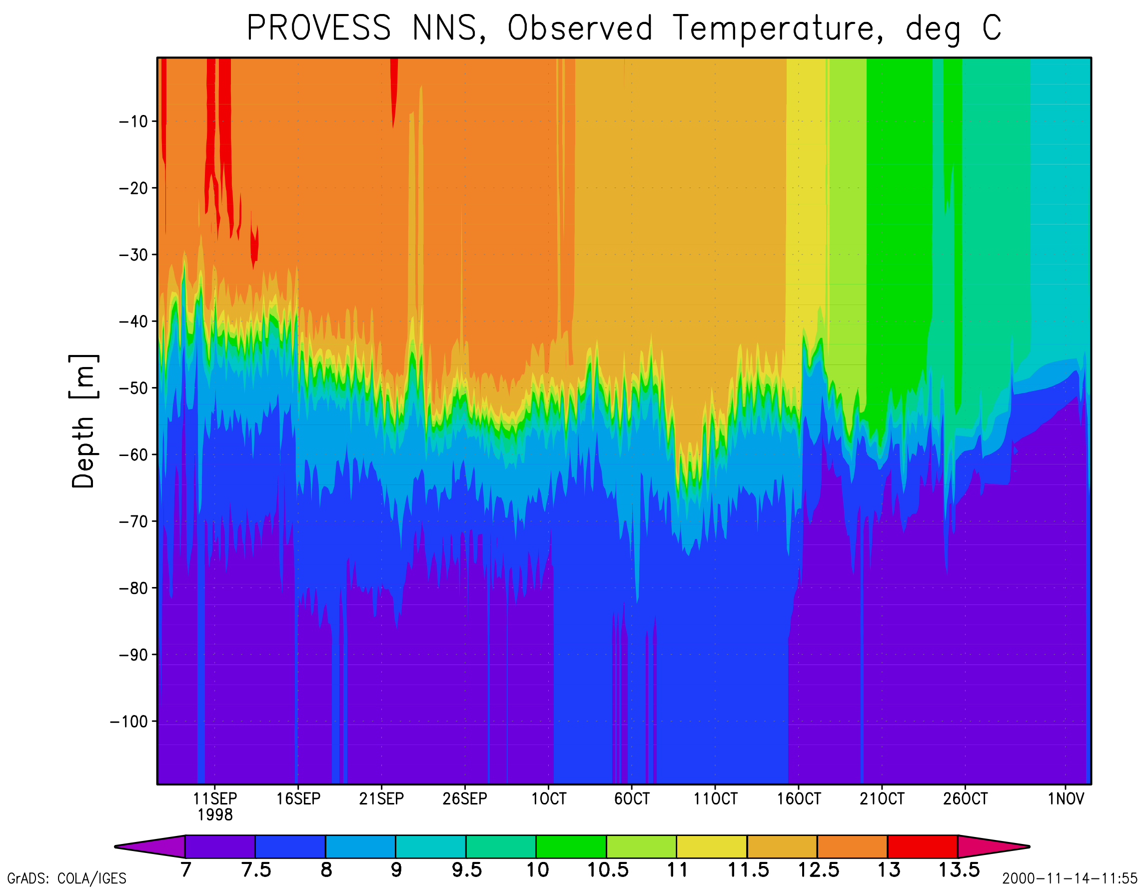
Wind and Tides



Burchard et al. [2002]

GOTM: Northern North Sea

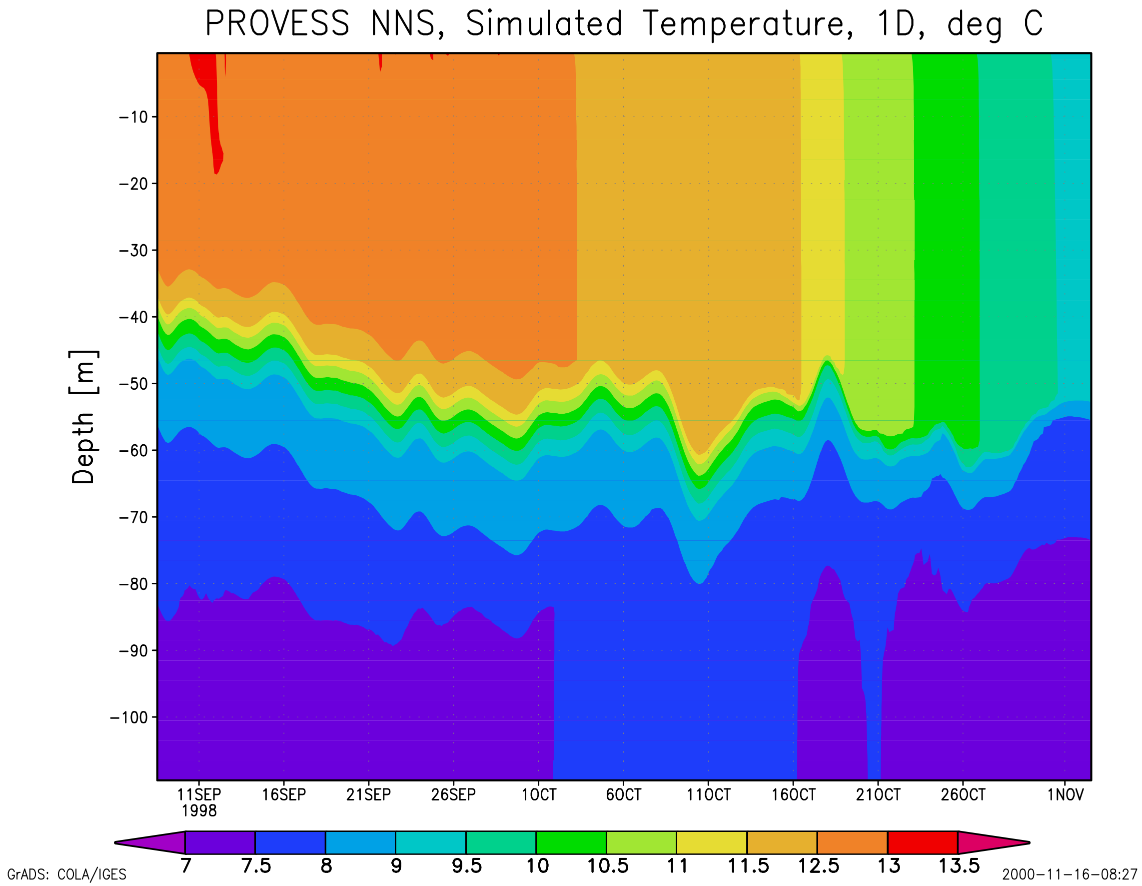
Observed temperature



Bolding et al. [2002]

GOTM: Northern North Sea

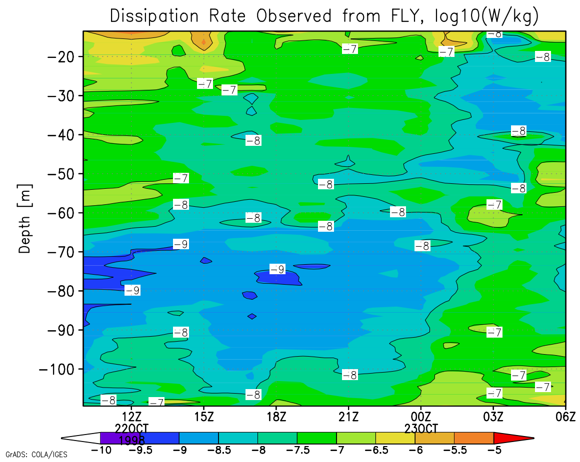
Simulated temperature

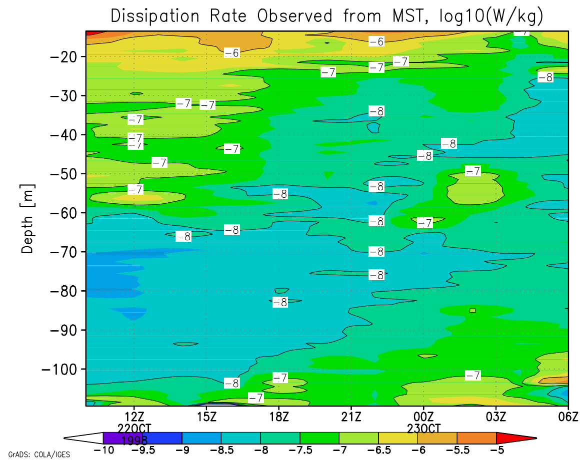


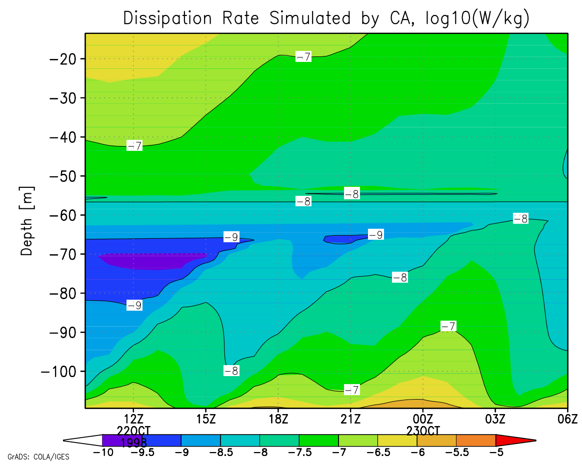
Bolding et al. [2002]

GOTM: Northern North Sea

Observed and simulated dissipation rate during 24 h:







Burchard et al. [2002]

NPZD model as example

Simple four-compartment model:

$$
\begin{aligned}
\mathcal{T}(N) &= -s_{NP} \quad +s_{PN} \quad +s_{ZN} \quad +s_{DN} \\
\mathcal{T}(P) &= +s_{NP} \quad -s_{PN} \quad -s_{PD} \quad -s_{PZ} \\
\mathcal{T}(Z) &= +s_{PZ} \quad -s_{ZN} \quad -s_{ZD} \\
\mathcal{T}(D) &= +s_{PD} \quad +s_{ZD} \quad -s_{DN}
\end{aligned}
$$

$$
\mathcal{T}(X) = \partial_t X - \partial_z(\nu_t' \partial_z X) - w_X \partial_z X
$$

From model physics

NPZD model as example

Phytoplankton nutrient uptake term:

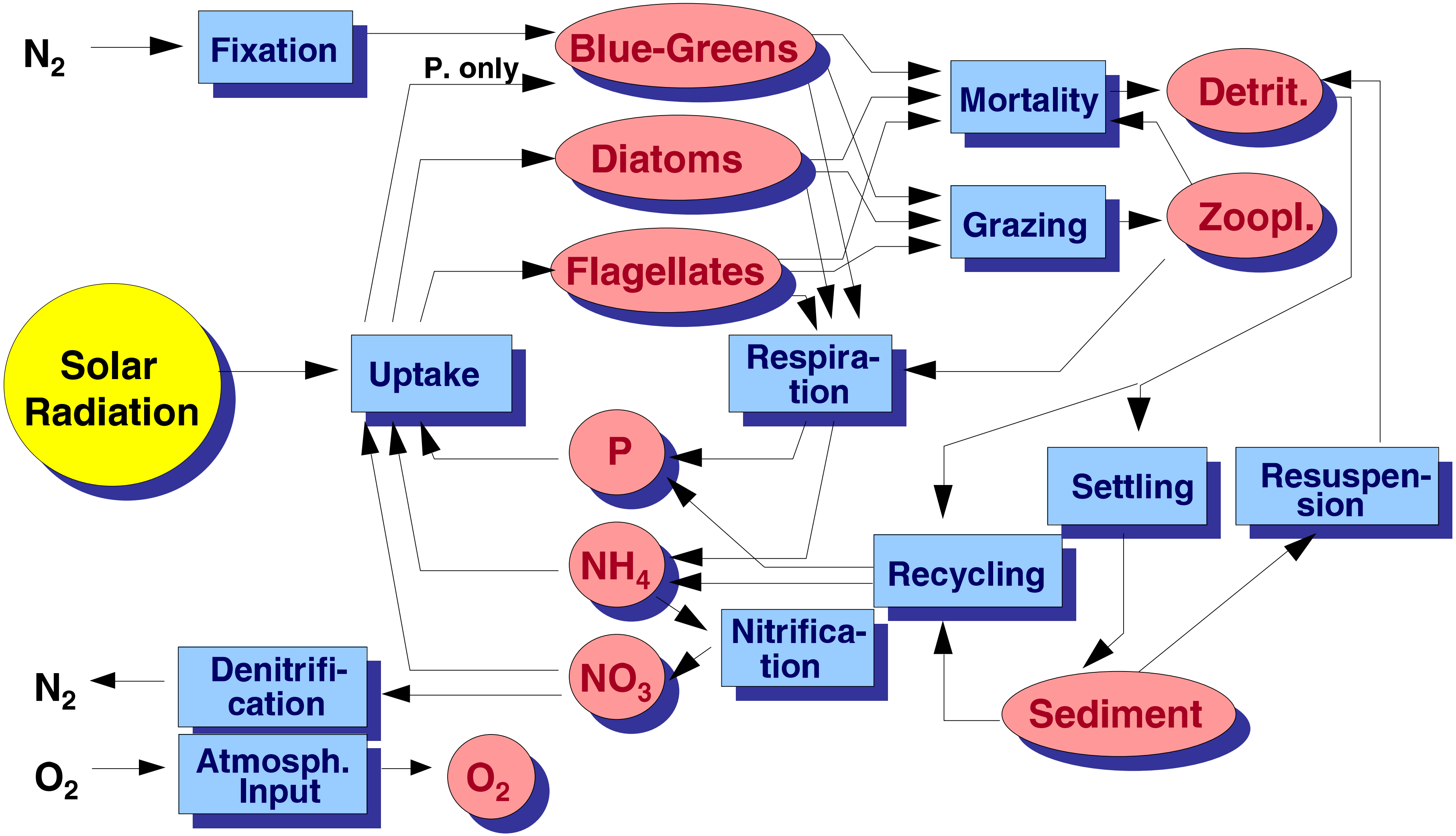
$$s_{NP} = \frac{I_{PAR}}{I_{opt}} \exp\left(1 - \frac{I_{PAR}}{I_{opt}}\right) \frac{N}{\alpha + N}(P + P_0)$$

$$I_{PAR}(z) = \frac{I_0}{2} \frac{a e^{-z/\eta_1} + (1-a) e^{-z/\eta_2}}{\exp\left(k_c \int_z^0 (P(\xi) + P_0 + D(\xi) + D_0)\, d\xi\right)}$$

From model physics

Back to model physics

IOW biogeochemical model



Neumann et al. [2002]

Positivity and conservation

Generic zero-dimensional model formulation:

$$d_t c_i = P_i(\vec{c}) - D_i(\vec{c}) \quad , i = 1, \dots, I, \tag{2}$$

$$\vec{c}^0 = \vec{c}(t=0) > \vec{0}, \tag{3}$$

$$P_i(\vec{c}) = \sum_{j=1}^{I} p_{i,j}(\vec{c}), \quad D_i(\vec{c}) = \sum_{j=1}^{I} d_{i,j}(\vec{c}), \tag{4}$$

$$p_{i,j}(\vec{c}) = d_{j,i}(\vec{c}), \quad \text{for } i \neq j. \tag{5}$$

Burchard et al. [2003]

Positivity and conservation

$$\sum_{i=1}^{I} (P_i(\vec{c}) - D_i(\vec{c})) = \qquad (6)$$

$$\sum_{i=1}^{I}\sum_{j=1}^{I} (p_{i,j}(\vec{c}) - d_{i,j}(\vec{c})) = \sum_{i=1}^{I} (p_{i,i}(\vec{c}) - d_{i,i}(\vec{c}))\,.$$

Thus, the system of equations is conservative for $p_{i,i} = d_{i,i} = 0$.

Burchard et al. [2003]

Positivity and conservation

Discretisation problems:

- Explicit schemes are conservative but not non-negative.
- Positive schemes are not necessarily conservative.

Problem: Find conservative and non-negative scheme.

Burchard et al. [2003]

Positivity and conservation

Solution, e.q. first order:

Modified Patankar-Euler scheme:

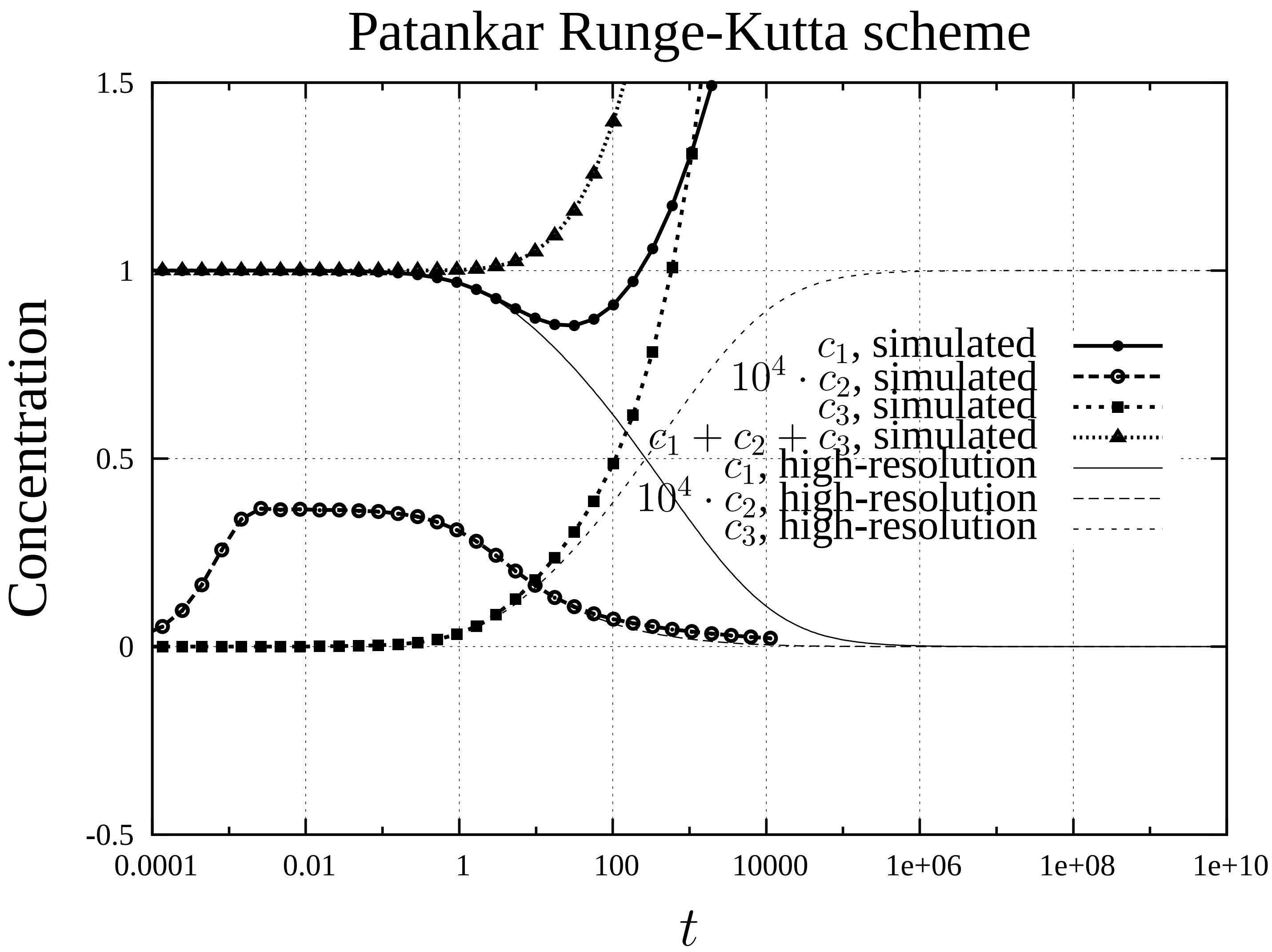
$$c_i^{n+1} = c_i^n + \Delta t \left(\sum_{j=1}^{I} p_{i,j}\left(\vec{c}^n\right) \frac{c_j^{n+1}}{c_j^n} - \sum_{j=1}^{I} d_{i,j}\left(\vec{c}^n\right) \frac{c_i^{n+1}}{c_i^n} \right), \quad i = 1, \ldots, \tag{7}$$

- The scheme is conservative (trivial)
- The scheme is non-negative (see *Burchard*, *Deleersnijder*, *Meister* [2003])

With the Runge-Kutta principle, conservative and non-negative schemes of arbitrary order may be constructed.

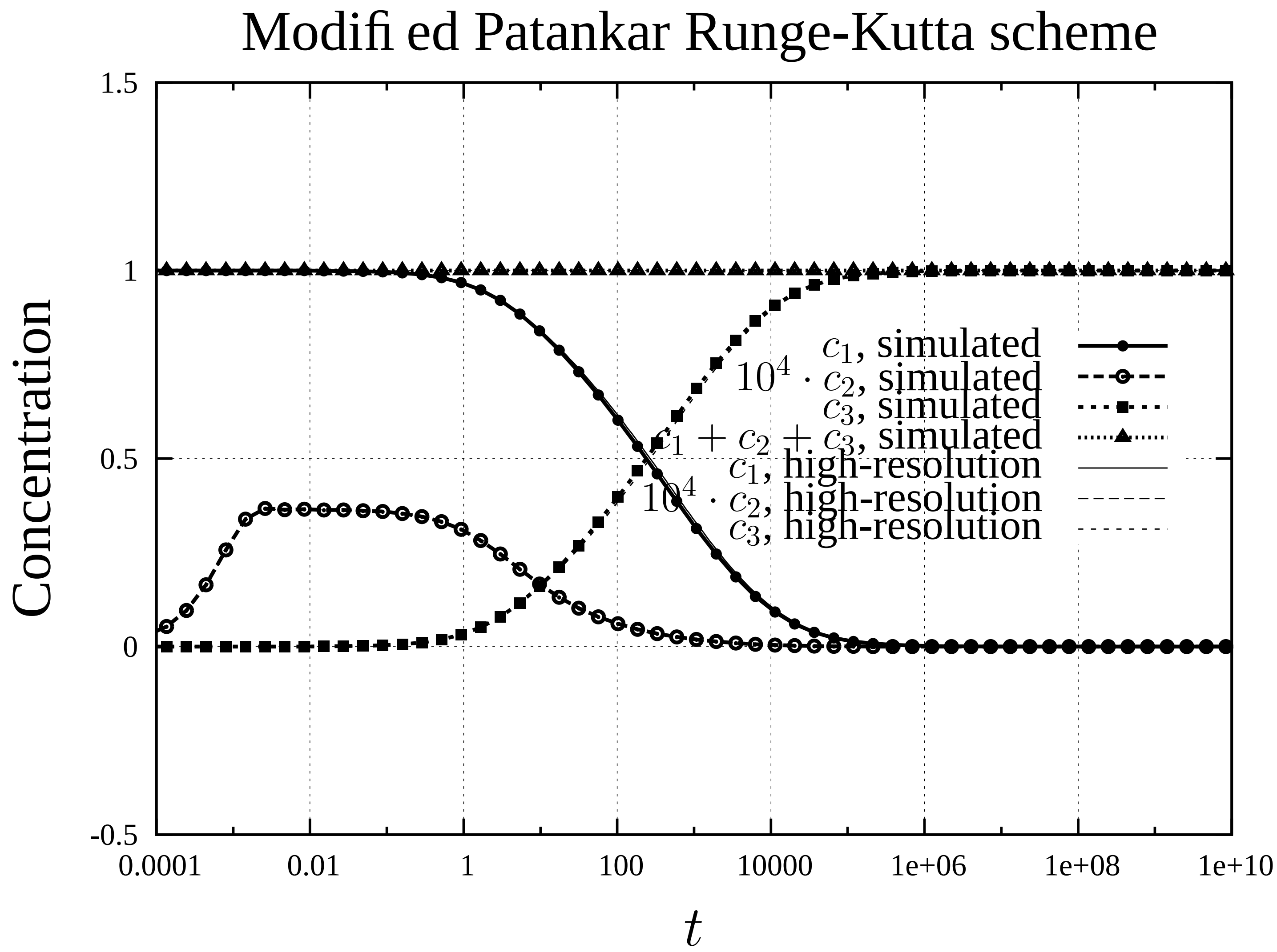
Burchard et al. [2003]

Positivity and conservation



Burchard et al. [2003]

Positivity and conservation



Burchard et al. [2003]

GOTM-BIO: principles

Principles for inclusion of various ecosystem models into GOTM:

- Only few well-defined interfaces between GOTM and BIO necessary:
  `init_bio(), do_bio(), end_bio()`
- BIO as two level system:
  1. General bio: setup is read from `bio.inp`
  2. Based on the chosen BIO-model, a second namelist is read in with model specific details
- Code must allow for various numerical methods for right-hand sides

GOTM-BIO: namelist input I

```
!------------------------------------------------------------------------
! Geobiochemical model
!
!  pelagic_calc=    .true.: calculate geobiochemical model
!  pelagic_model=
!                 1: NPZD
!                 2: IOW
!  w_adv_discr= advection scheme for vertical motion
!                 2: first order upstream
...
!                 6: TVD with ULTIMATE QUICKEST
!  ode_method=   scheme for source & sink dynamics
!                 1: first-order explicit (not positive)
...
!                 8: mod. Patankar-RK scheme (second ord., positive, conservative)
!                 9: mod. Patankar-RK scheme (fourth ord., positive, conservative)
!------------------------------------------------------------------------
&pelagic_nml
  pelagic_calc=.true.,
  pelagic_model=2
  ode_method=1,
  w_adv_discr=6,
```

GOTM-BIO: namelist input II

```
!---------------------------------------------------------------------------
! NPZD biological model
!
!  numc=         number of compartments for geobiochemical model
!  n_initial=    initial nutrient concentration                    [mmol N/m**3]
!  p_initial=    initial phytoplankton concentration               [mmol N/m**3]
!  z_initial=    initial zooplankton concentration                 [mmol N/m**3]
!  d_initial=    initial detritus concentration                    [mmol N/m**3]
!  p0=           minimum phytoplankton concentration (to be added to p)  [ " ]
!  z0=           minimum zooplankton concentration (to be added to z)    [ " ]
!  w_p=          settling velocity of phytoplankton                [m/d]
!  w_d=          settling velocity of zooplankton                  [m/d]
!  kc=           attenuation constant for the self shading effect  [m**2/mmol N]
!  I_min=        minimum photosynthetically active radiation (PAR) [W/m**2]
!  rmax=        maximum nutrient uptake rate                       [1/d]
!  gmax=         maximum grazing rate                              [1/d]
!  Iv=           Ivlev constant                                    [ - ]
!  alpha=        half saturation                                   [mmol N/m**3]
!  rpn=          p --> n rate (p metabolism)                       [1/d]
!  rzn=          z --> n rate (z metabolism)                       [1/d]
!  rdn=          d --> n rate (remineralisation)                   [1/d]
!  rpdu=         p --> d rate (p mortality), in euphotic zone      [1/d]
!  rpdl=         p --> d rate (p mortality), below euphotic zone   [1/d]
!  rzd=          z --> d rate (z mortality)                        [1/d]
!  cnpar=        Crank-Nickolson parameter fo vertical diffusion
!---------------------------------------------------------------------------
```

GOTM-BIO: code I

```
#ifdef PELAGIC
    call do_pelagic(nlev,I_0,dt,h,t,nuh,rad,bioshade)
#endif
```

`nlev`	for	number of vertical layers,
`I_0`	for	net shortwave radiation at surface,
`dt`	for	Δt,
`h`	for	layer heights,
`t`	for	potential temperature in each layer,
`nuh`	for	eddy diffusivity at each layer interface,
`rad`	for	net shortwave radiation at each interface,
`bioshade`	for	turbidity due to organic material.

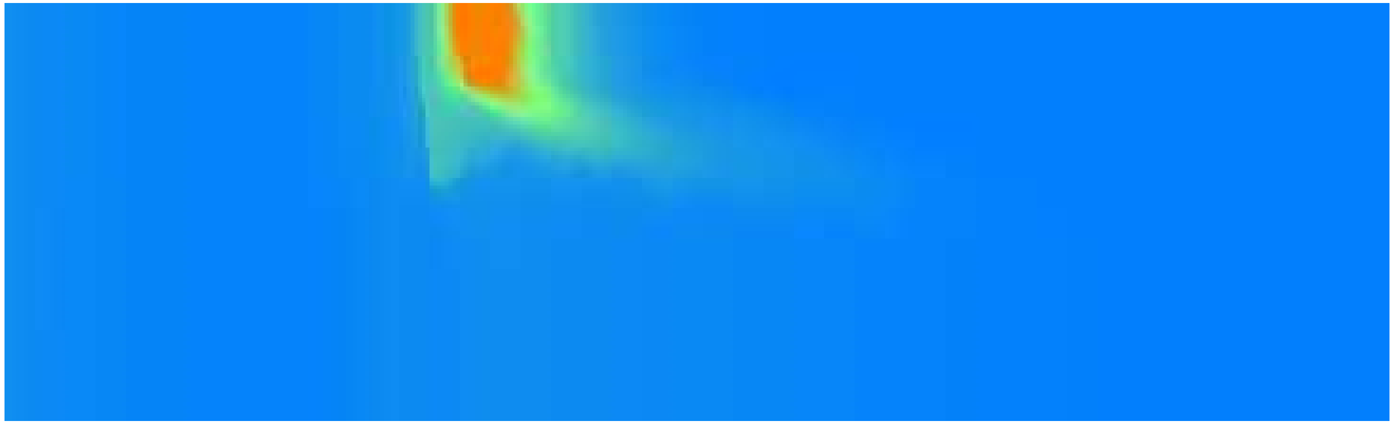
GOTM-BIO: code for NPZD

```
do ci=1,nlev
   dd(n,p,ci)=fnp(cc(n,ci),cc(p,ci),par(ci),iopt)
   dd(p,z,ci)=fpz(cc(p,ci),cc(z,ci))
   dd(p,n,ci)=rpn*cc(p,ci)
   dd(z,n,ci)=rzn*cc(z,ci)
   dd(d,n,ci)=rdn*cc(d,ci)
   dd(p,d,ci)=rpd*cc(p,ci)
   dd(z,d,ci)=rzd*cc(z,ci)
   do i=1,numc
      do j=1,numc
         pp(i,j,ci)=dd(j,i,ci)
      end do
   end do
end do
```

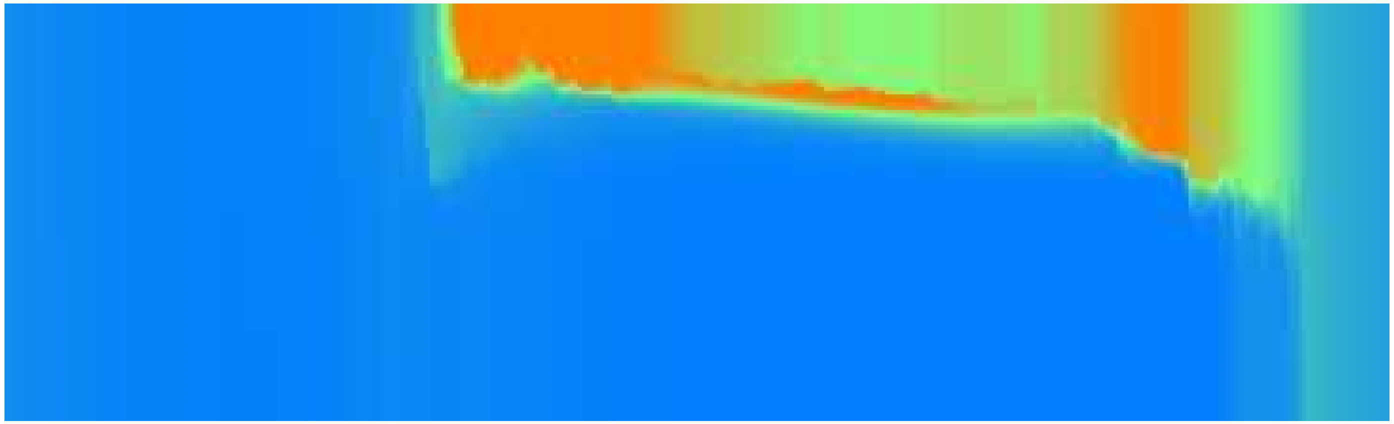
GOTM Example: IOW model

Application to Northern North Sea as before.

Diatoms (min: 0 mmol N/m^3, max: 1.5 mmol N/m^3):



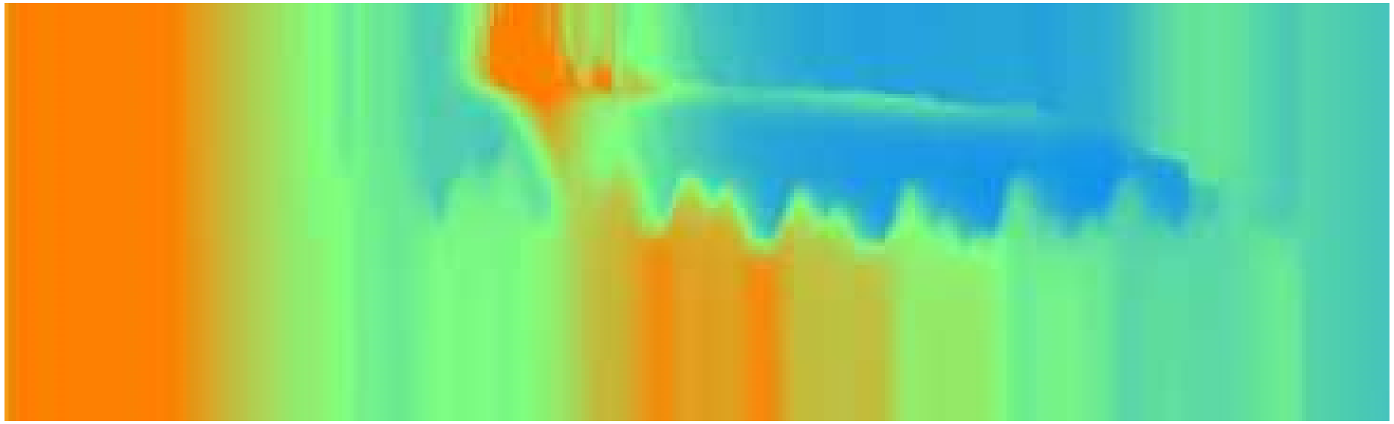
Flagellates (min: 0 mmol N/m^3, max: 1.5 mmol N/m^3):



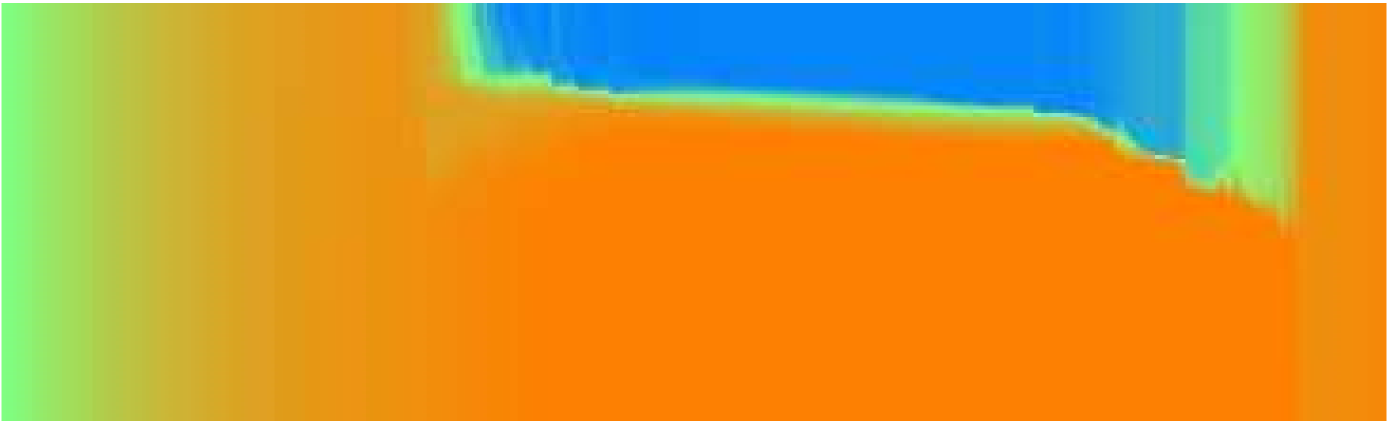
GOTM Example: IOW model

Application to Northern North Sea as before.

Ammonium (min: 0 mmol N/m^3, max: 0.2 mmol N/m^3):



Nitrate (min: 0 mmol N/m^3, max: 10 mmol N/m^3):



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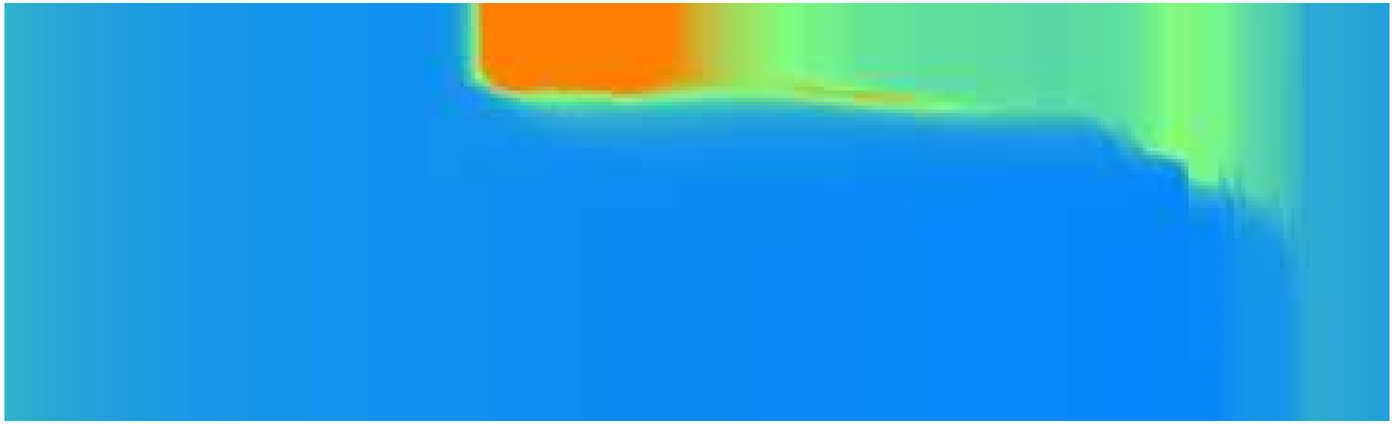
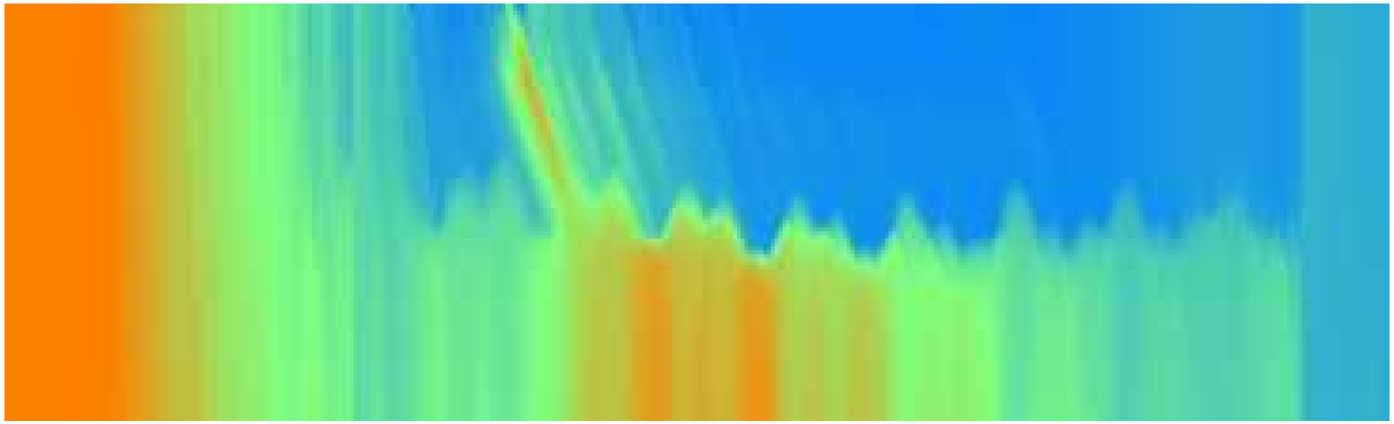
GOTM Example: IOW model

Application to Northern North Sea as before.

Zooplankton (min: 0 mmol N/m^3, max: 0.5 mmol N/m^3):



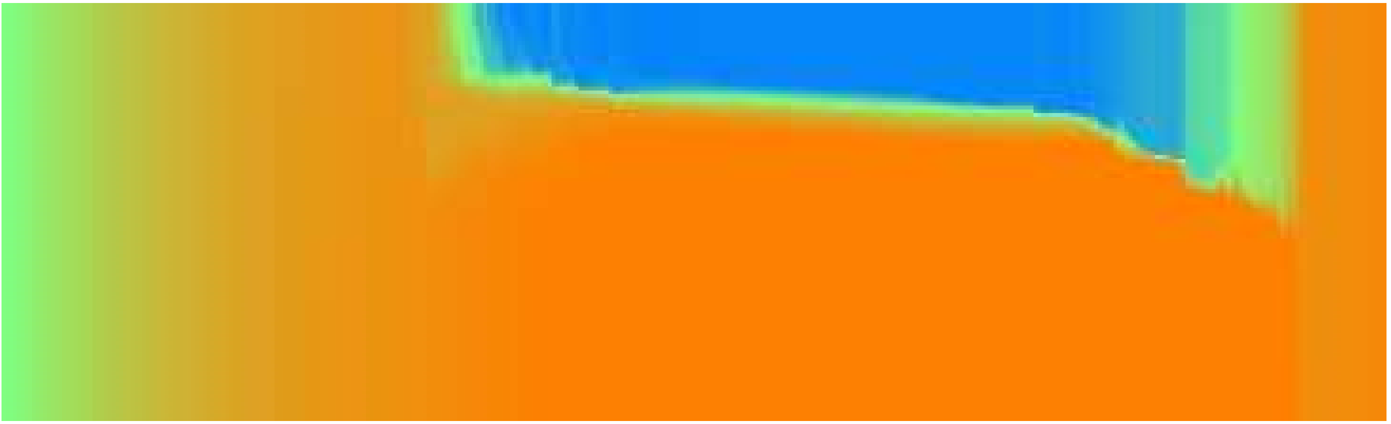
Detritus (min: 0 mmol N/m^3, max: 3 mmol N/m^3):



GOTM Example: IOW model

Application to Northern North Sea as before.

Oxygen (min: 300 $mmol/m^3$, max: 380 $mmol/m^3$):



Road map towards GOTM-BIO

1. Try to get funded
2. Implement some more ecosystem models in GOTM (e.g. *Fasham* [1990])
3. Create scenarios suitable for ecosystem model comparison (e.g. FLEX, ESTOC, OWS PAPA)
4. Generate Windows version for GOTM
5. Write documentation & user guide
6. Write scientifi c paper on model comparison with GOTM-BIO
7. Release GOTM-BIO
8. Get flooded with email requests from biologists