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

Hans Burchard\textsuperscript{1,2,3}, Karsten Bolding\textsuperscript{2,3}, Thomas Neumann\textsuperscript{1}, Wolfgang Fennel\textsuperscript{1}, Torsten Seifert\textsuperscript{1}, Lars Umlauf\textsuperscript{1,3}, and Marie Maar\textsuperscript{2}

1. Baltic Sea Research Institute Warnemünde, Germany
2. Bolding & Burchard Hydrodynamics, Denmark/Germany
3. Member of GOTM Team, \url{http://www.gotm.net}
Contents

• 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.

⇒ They can only be compared to each others in identical physical frames.

⇒ 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 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.
GOTM: Algebraic SMCs

Turbulent Fluxes:

\[ \langle \bar{u} \bar{w} \rangle = -\nu_t \partial_z \bar{u}, \quad \langle \bar{w} \bar{T} \rangle = -\nu'_t \partial_z \bar{T} \]

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

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

\[ L \propto \frac{k^{3/2}}{\varepsilon} \]  \hspace{1cm} (1)

- \( k \) \hspace{1cm} \text{turbulent kinetic energy}
- \( P \) \hspace{1cm} \text{shear production}
- \( B \) \hspace{1cm} \text{buoyancy production}
- \( \varepsilon \) \hspace{1cm} \text{viscous dissipation}
- \( L \) \hspace{1cm} \text{macro length scale}
GOTM: Length scale equations

$k-\varepsilon$ 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]):

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

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

$k$-$\omega$ model (Wilcox [1988], Umlauf et al. [2003]):

\[ \partial_t \omega - \partial_z \left( \frac{\nu_t}{\sigma_\omega} \partial_z \omega \right) = \frac{\omega}{k} (c_{m1} P + c_{m3} B - c_{m2} \varepsilon), \quad \omega = \frac{\varepsilon}{k}. \]

Generic model (Umlauf and Burchard [2003]):

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

\[ k^{m-1} L^n (c_{nm1} P + c_{mn3} B - c_{mn2} \varepsilon). \]
GOTM: Northern North Sea

Bathymetry and station map

Burchard et al. [2002]
GOTM: Northern North Sea

Wind and Tides

Surface stress at station NNS

Bed stress at station NNS

Date in 1998

Burchard et al. [2002]
GOTM: Northern North Sea

Observed temperature

PROVESS NNS, Observed Temperature, deg C

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:

\[ T(N) = -s_{NP} + s_{PN} + s_{ZN} + s_{DN} \]
\[ T(P) = +s_{NP} - s_{PN} - s_{PD} - s_{PZ} \]
\[ T(Z) = +s_{PZ} - s_{ZN} - s_{ZD} \]
\[ T(D) = +s_{PD} + s_{ZD} - s_{DN} \]

\[ T(X) = \partial_t X - \partial_z (\nu_t' \partial_z X) - w_X \partial_z X \]

From model physics
NPZD model as example

Phytoplankton nutrient uptake term:

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

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

From model physics
Back to model physics
IOW biogeochemical model

Neumann et al. [2002]
Positivity and conservation

Generic zero-dimensional model formulation:

\[ d_t c_i = P_i(c) - D_i(c) \quad , \quad i = 1, \ldots , I , \]  \hspace{1cm} (2)

\[ c^0 = c(t = 0) > \bar{0} , \]  \hspace{1cm} (3)

\[ P_i(c) = \sum_{j=1}^{I} p_{i,j}(c) , \quad D_i(c) = \sum_{j=1}^{I} d_{i,j}(c) , \]  \hspace{1cm} (4)

\[ p_{i,j}(c) = d_{j,i}(c) , \quad \text{for} \quad i \neq j . \]  \hspace{1cm} (5)

Burchard et al. [2003]
Positivity and conservation

\[
\sum_{i=1}^{I} (P_i(\vec{c}) - D_i(\vec{c})) = 
\]

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

Thus, the system of equations is **conservative** for \( p_{i,i} = d_{i,i} = 0 \).

*Burchard et al. [2003]*
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:

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

(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.
Positivity and conservation

Patankar Runge-Kutta scheme

\begin{align*}
\text{Concentration} = & \ c_1, \text{simulated} \\
\text{Concentration} = & \ c_2, \text{simulated} \\
\text{Concentration} = & \ c_3, \text{simulated} \\
\text{Concentration} = & \ c_1, \text{high-resolution} \\
\text{Concentration} = & \ c_2, \text{high-resolution} \\
\text{Concentration} = & \ c_3, \text{high-resolution}
\end{align*}

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:
  
  \begin{verbatim}
  init_bio(), do_bio(), end_bio()
  \end{verbatim}

- 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 for vertical diffusion
!-------------------------------------------------------------------------------
GOTM-BIO: code I

```c
#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 $\Delta t$,
- `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$^3$):

![Diatoms concentration map]

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

![Flagellates concentration map]
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$^3$):
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 scientific paper on model comparison with GOTM-BIO
7. Release GOTM-BIO
8. Get flooded with email requests from biologists