Patankar-type positive-definite and conservative solvers for reactive terms in biogeochemical models

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Research Problem

Biogeochemical models are typically based on nutrient equivalents, which are basically conserved inside the system. The state variables are expressed as non-negative concentrations.

However, typical numerical solvers for biogeochemical models are either non-positive or non-conservative.

Here, a non-negative and conservative discretisation is introduced.

Ecosystem models

The general structure of an ecosystem model is given as the following set of equations:

$$\partial_t c_i + \partial_j (u_j c_i + m_j c_i - A_{j,k} \partial_k c_i) = P_i(\vec{c}) - D_i(\vec{c}), \quad i = 1, \ldots, I, \tag{1}$$

c_i	concentrations
u_j	current velocity
m_j	motion of ecosystem component
$A_{j,k}$	eddy diffusivity
$P_i(\vec{c}), D_i(\vec{c})$	source & sink terms

Ecosystem models

Often, transport and reactions are calculated separately. The reaction part alone is described as system of ordinary differential equations:

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

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

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

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

Ecosystem models

All non-conservative sinks & sources (e.g. nitrogen fixation) are lumped together into the diagonal terms $p_{i,i}$ and $d_{i,i}$. For zero diagonal terms, conservation is easily seen:

$$d_t\left(\sum_{i=1}^{I} c_i\right) = \sum_{i=1}^{I}\left(P_i(\vec{c}) - D_i(\vec{c})\right) =$$

$$\sum_{i=1}^{I}\sum_{j=1}^{I}\left(p_{i,j}(\vec{c}) - d_{i,j}(\vec{c})\right) = \sum_{i=1}^{I}\left(p_{i,i}(\vec{c}) - d_{i,i}(\vec{c})\right). \quad (6)$$

Modelling problems

Concentrations are by definition non-negative quantities. Typical causes for negative concentrations in ecosystem models (often accompanied by numerical model blow-ups) are:

1. Mathematical formulation allows for negative concentrations (positive sinks even for zero concentration)
2. Non-monotone advection schemes are used (e.g. central differences)
3. Solvers for ODEs are non-positive (e.g. Euler-forward)

Solutions to problem 1

Problem 1: Mathematical formulation allows for negative concentrations (positive sinks even for zero concentration).

Solution: Formulate the sinks properly:

$$d_{i,j}(\vec{c}) \longrightarrow 0 \ \text{ for } \ c_i \longrightarrow 0 \tag{7}$$

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Solutions to problem 2

Problem 2: Non-monotone advection schemes are used (e.g. central differences).

Solution: Use monotone advection schemes such as

- First-order upstream (too diffusive)
- TVD (Total Variation Diminishing) schemes
- Flux-corrected transport schemes

Solutions to problem 3

Problem 3: Solvers for ODEs are non-positive (e.g. Euler-forward).

Solutions:

- Use sufficiently small time step (difficult to predict, often too expensive)
- Use adaptive time steps (often too expensive)
- Use non-negative schemes (often not conservative, **topic of this presentation**)

Euler-forward

$$c_i^{n+1} = c_i^n + \Delta t \left(P_i \left(\vec{c}^n \right) - D_i \left(\vec{c}^n \right) \right). \qquad (8)$$

Conservative but NOT non-negative.

Patankar-Euler scheme

$$c_i^{n+1} = c_i^n + \Delta t \left(P_i\left(\vec{c}^n\right) - D_i\left(\vec{c}^n\right) \frac{c_i^{n+1}}{c_i^n} \right). \qquad (9)$$

Non-negative but NOT conservative.

mod. Patankar-Euler scheme

$$c_i^{n+1} = c_i^n + \Delta t \left(\sum_{j=1}^{I} p_{i,j} \left(\vec{c}^n \right) \frac{c_j^{n+1}}{c_j^n} - \sum_{j=1}^{I} d_{i,j} \left(\vec{c}^n \right) \frac{c_i^{n+1}}{c_i^n} \right). \tag{10}$$

Burchard, Deleersnijder and Meister, Appl. Numer. Math., 2003.

Conservative AND non-negative
(but a linear system of equations has to be solved)

Second order schemes

The three schemes may also be extended to second order Runge-Kutta schemes:

- Runge-Kutta scheme
- Patankar-Runge-Kutta scheme
- Modified Patankar-Runge-Kutta scheme

Higher order schemes should also be constructable.

Simple linear model

$$\begin{aligned} d_t c_1 &= c_2 - a c_1, \\ d_t c_2 &= a c_1 - c_2, \end{aligned} \tag{11}$$

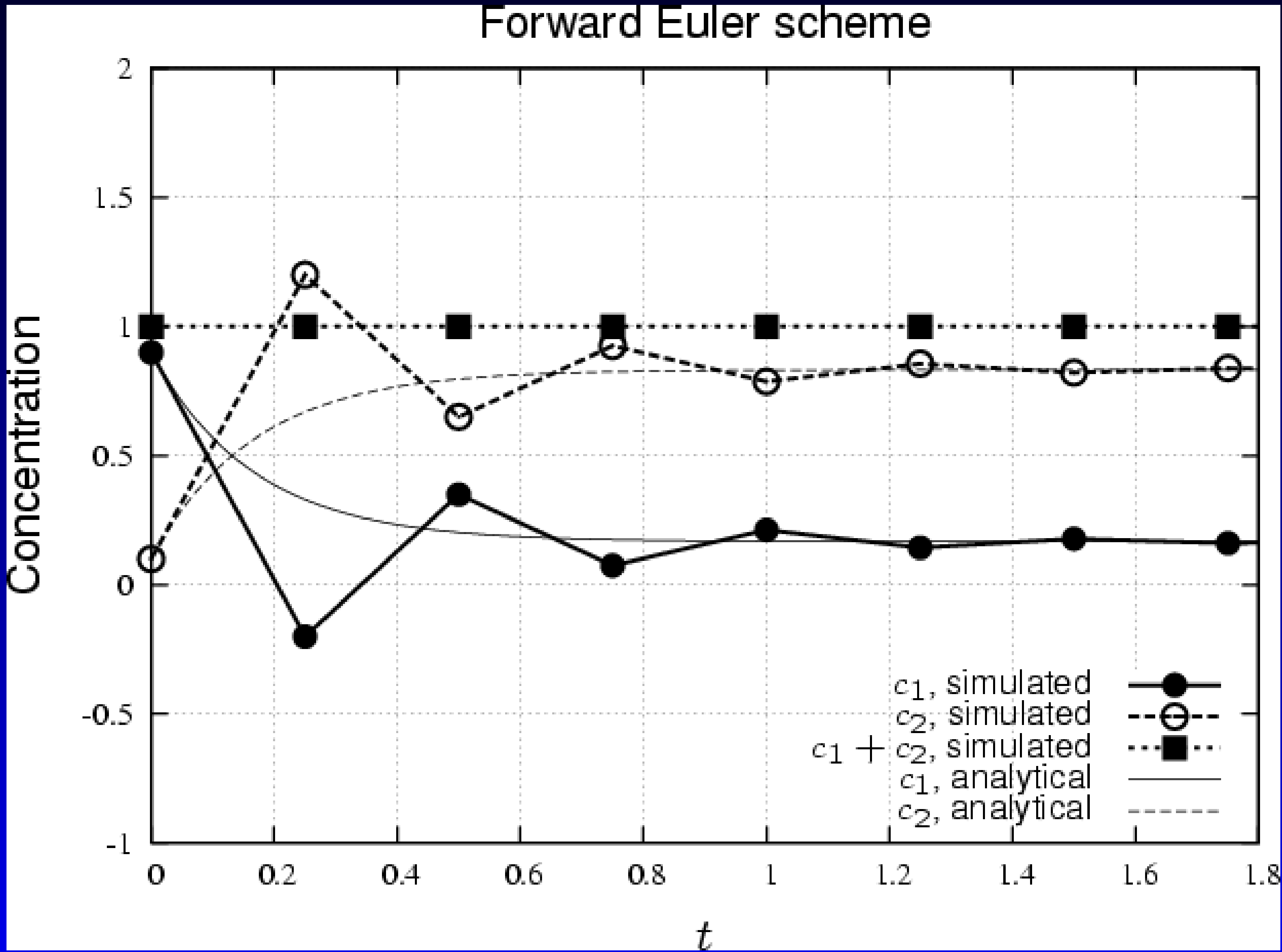
Analytical solution:

$$c_1 = \left(1 + c \exp\left(-(a+1)t\right)\right) c_1^\infty, \tag{12}$$

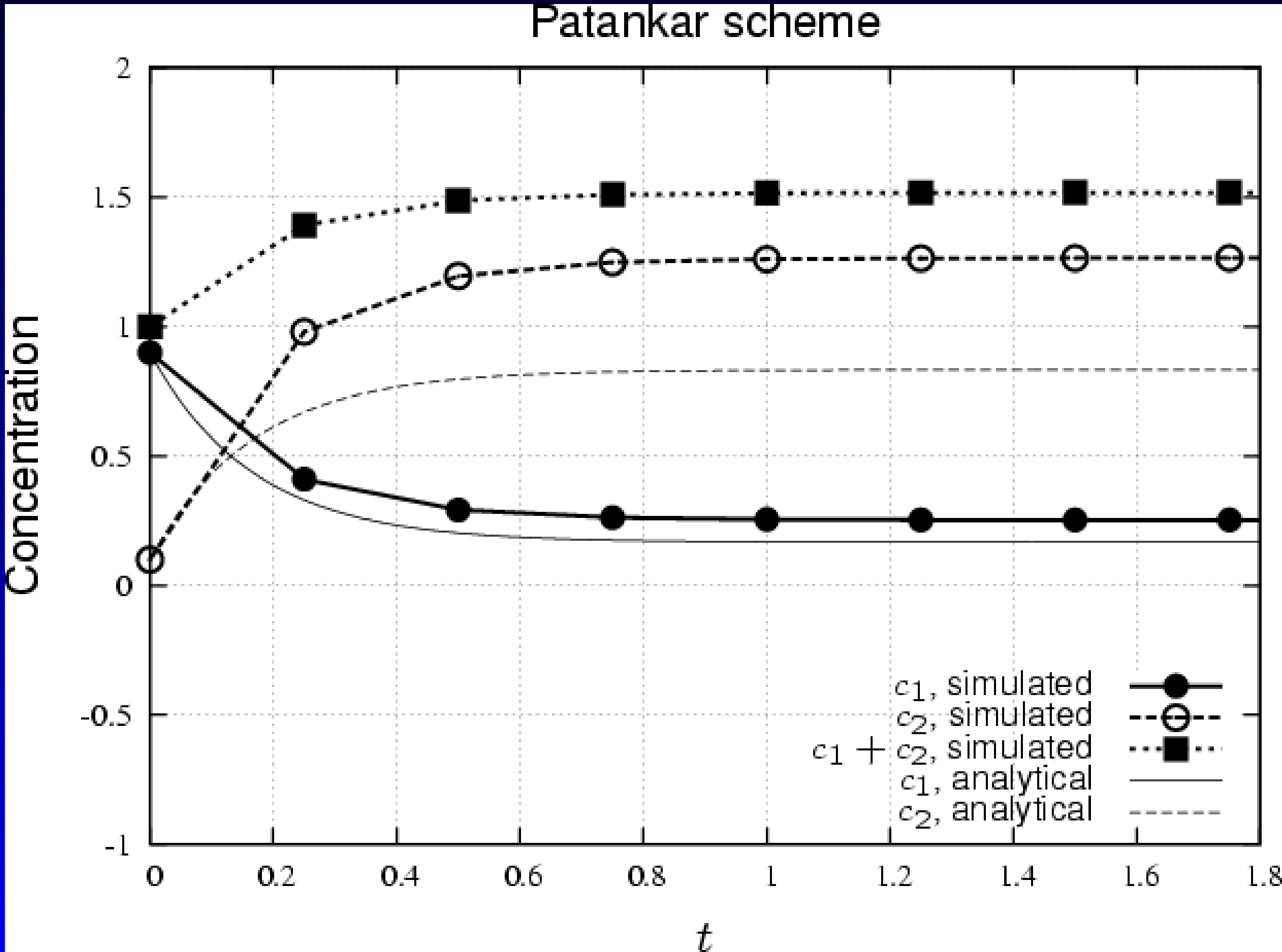
$$c_1^\infty = \frac{c_1^0 + c_2^0}{a+1} \quad \text{and} \quad c = \frac{c_1^0}{c_1^\infty} - 1. \tag{13}$$

(Here: $a = 5$, $c_1^0 = 0.9$, $c_2^0 = 0.1$)

Euler-forward



Patankar-Euler



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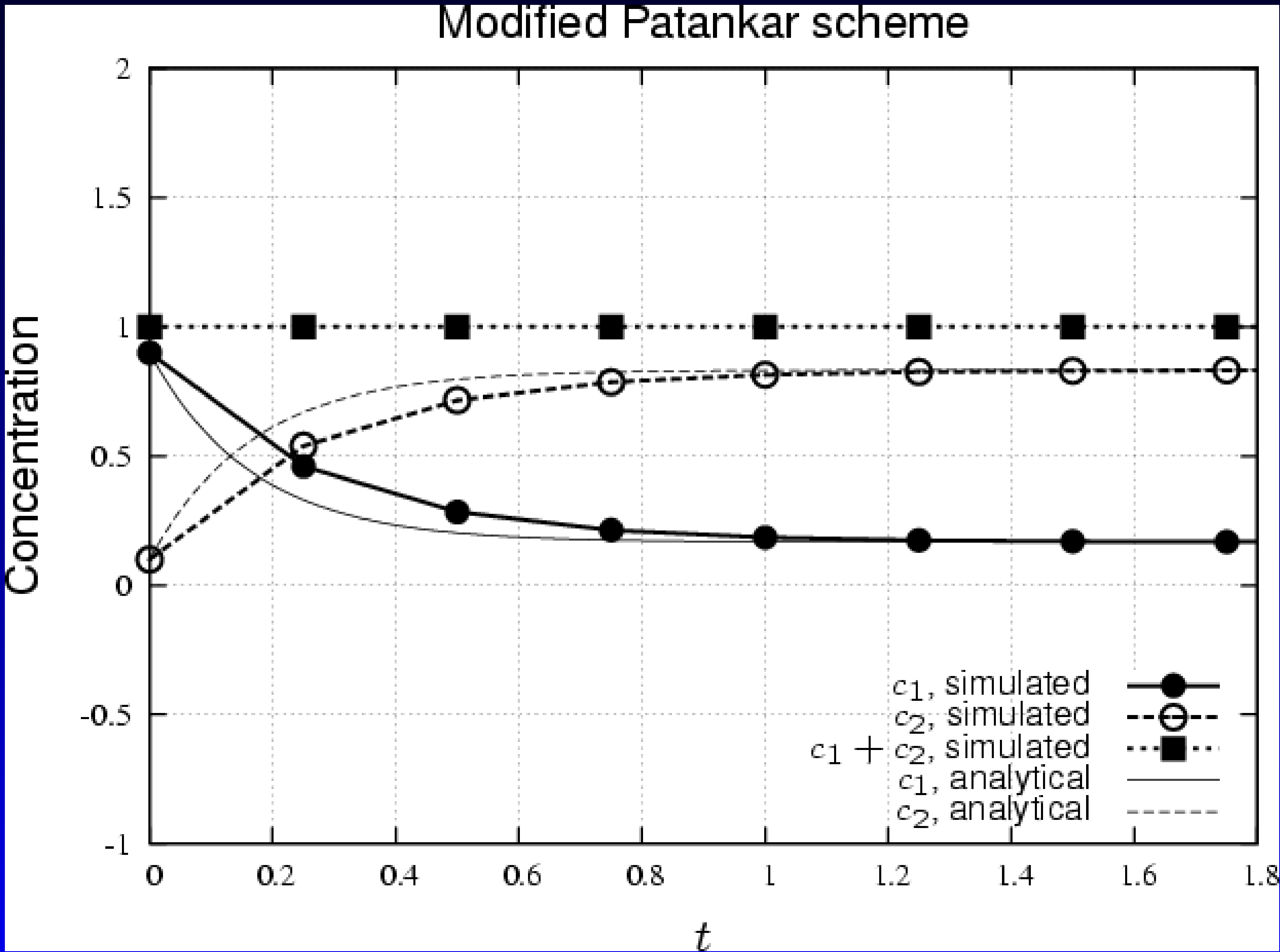
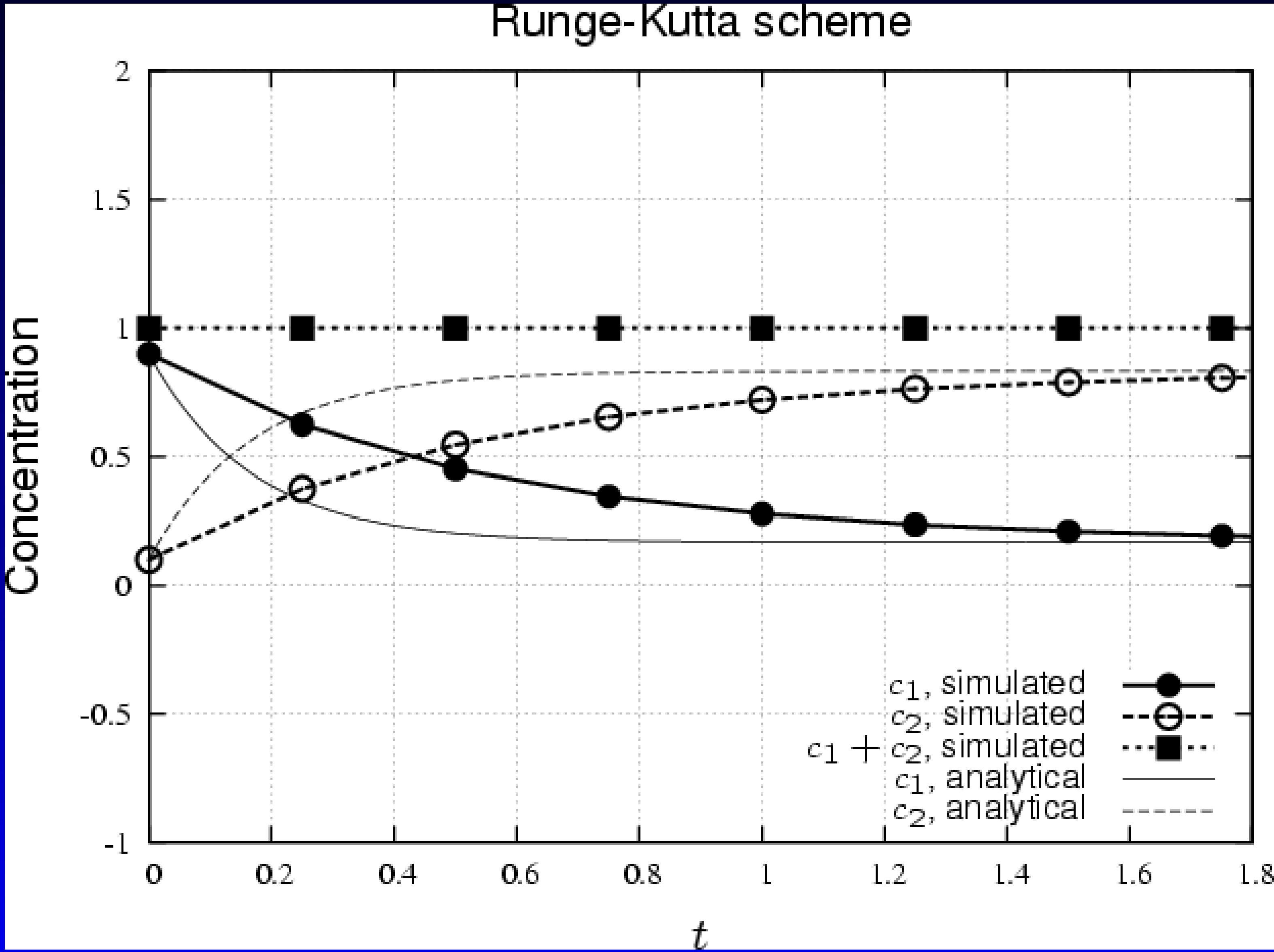
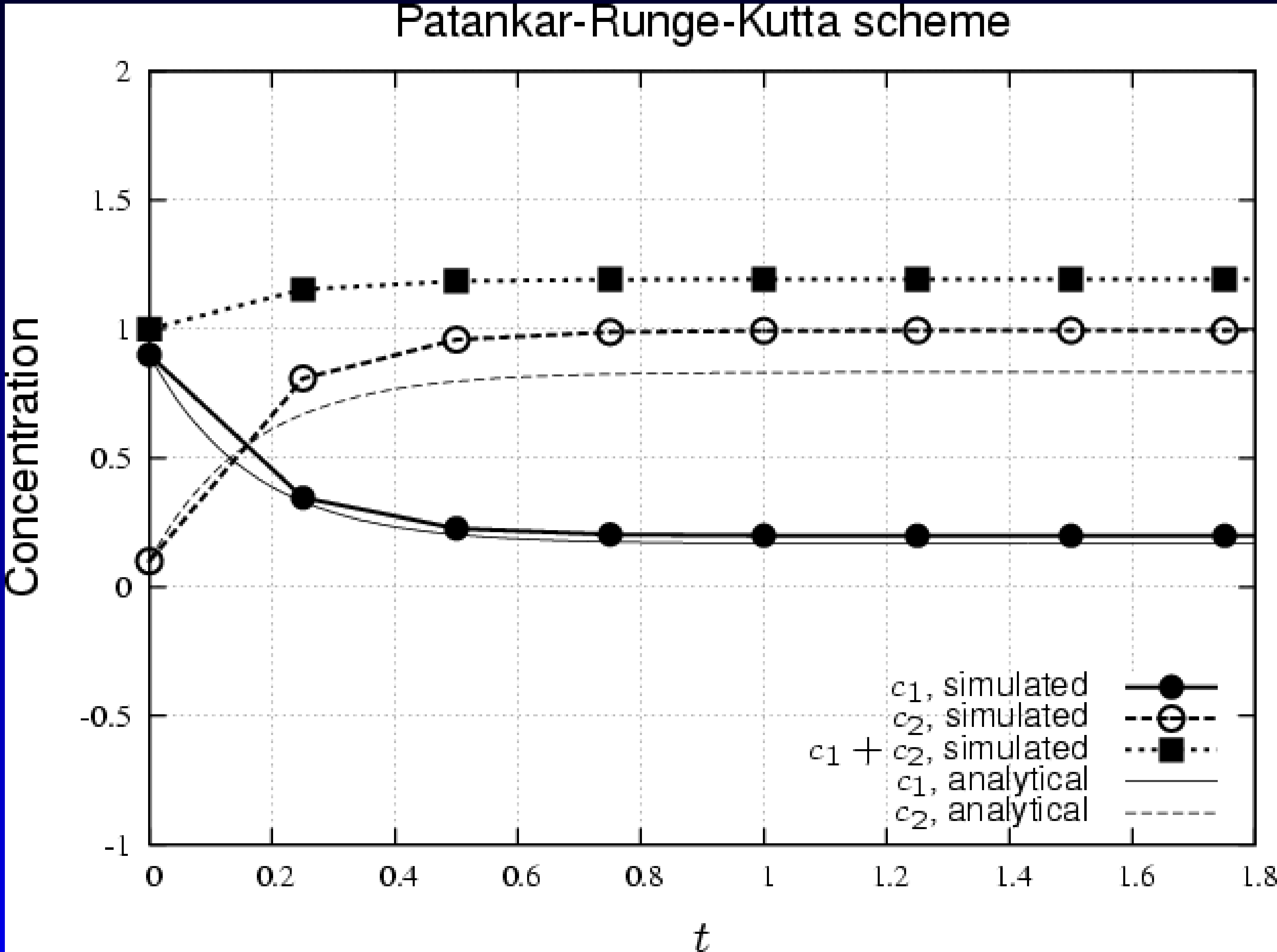
mod. Patankar-Euler



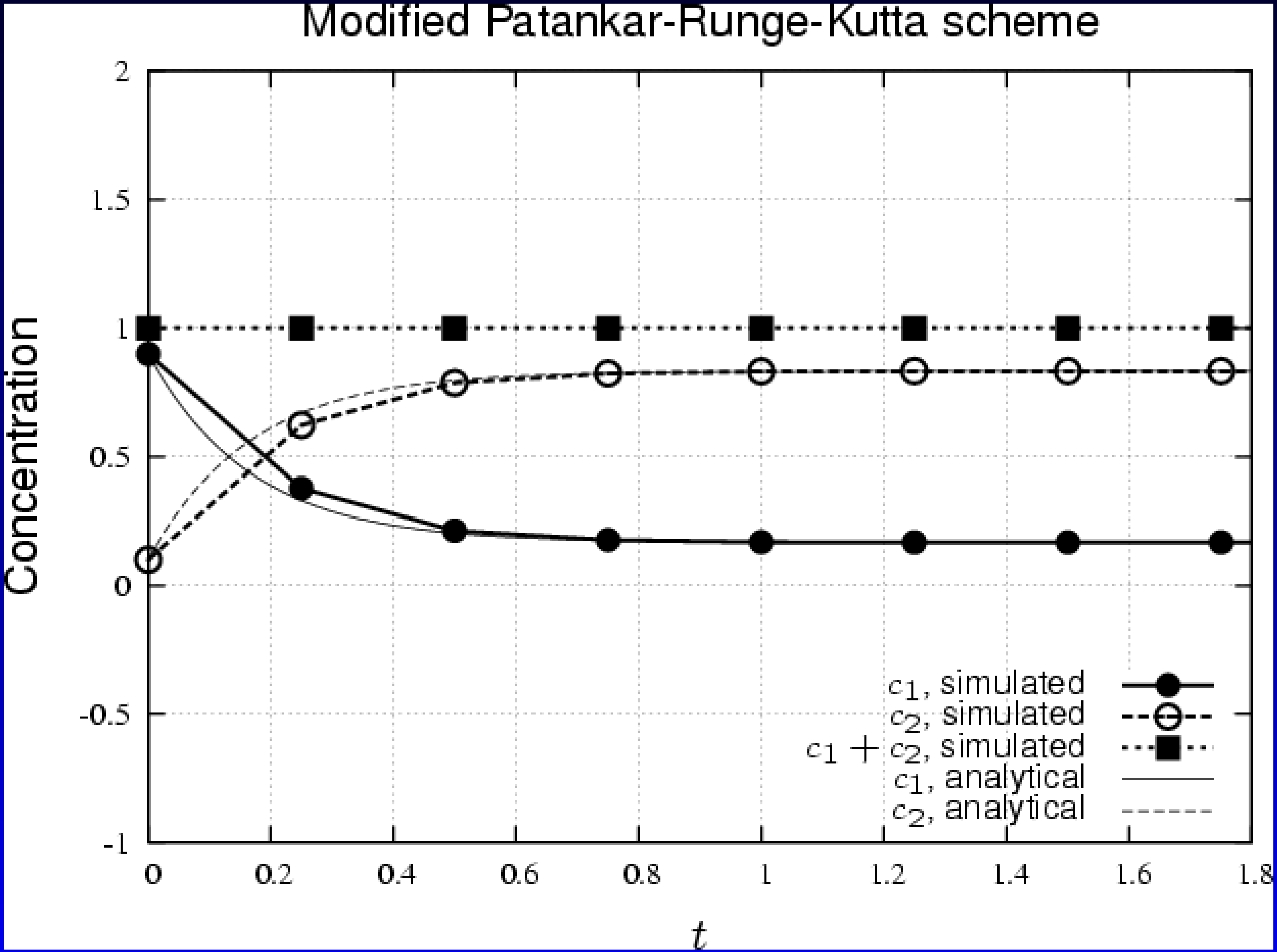
Runke-Kutta


Runge-Kutta scheme
Concentration
t
2
1.5
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
c_1, simulated
c_2, simulated
$c_1 + c_2$, simulated
c_1, analytical
c_2, analytical

Patankar-Runge-Kutta



mod. Patankar-Runge-Kutta



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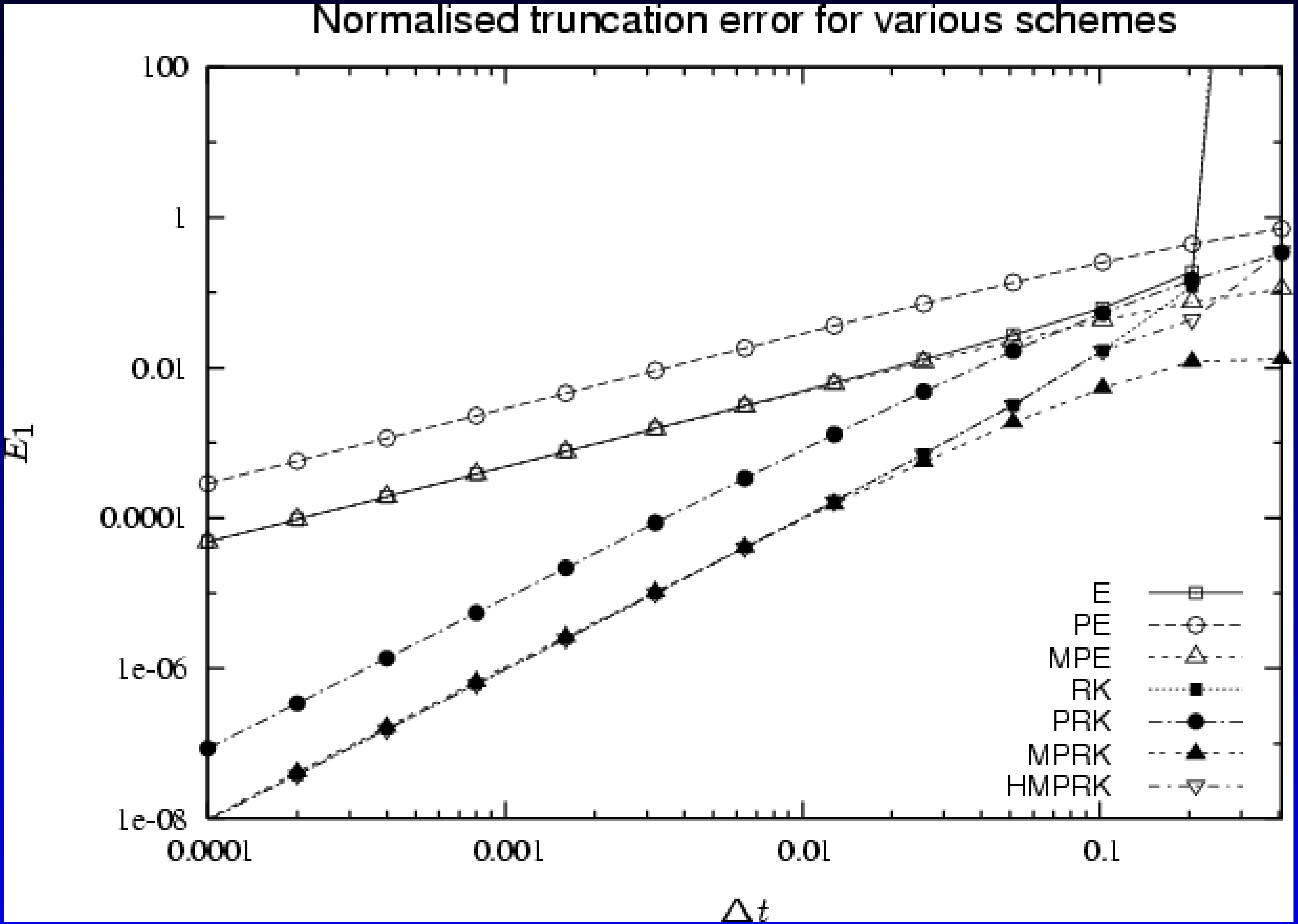
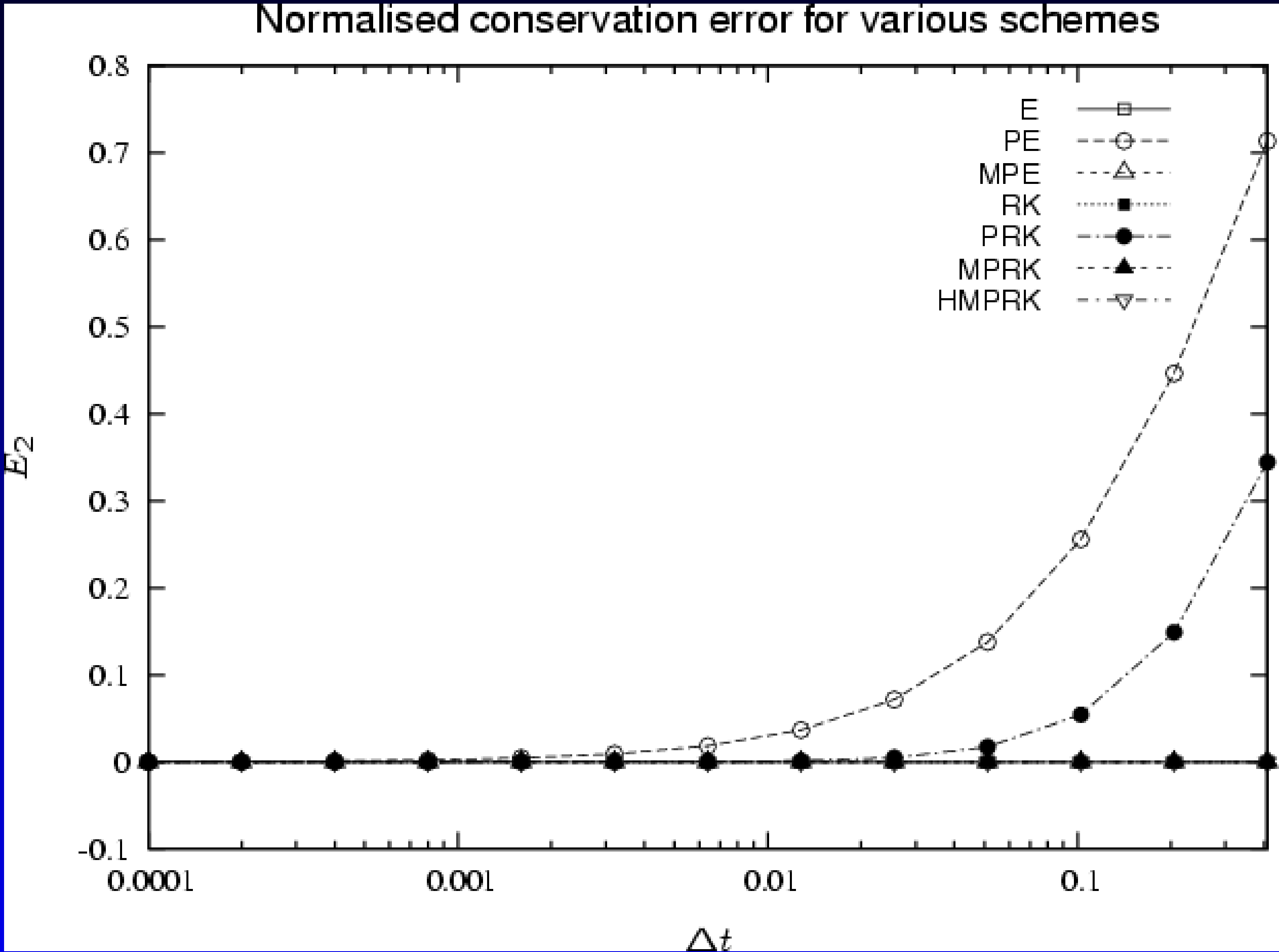
Approximation error



Conservation error



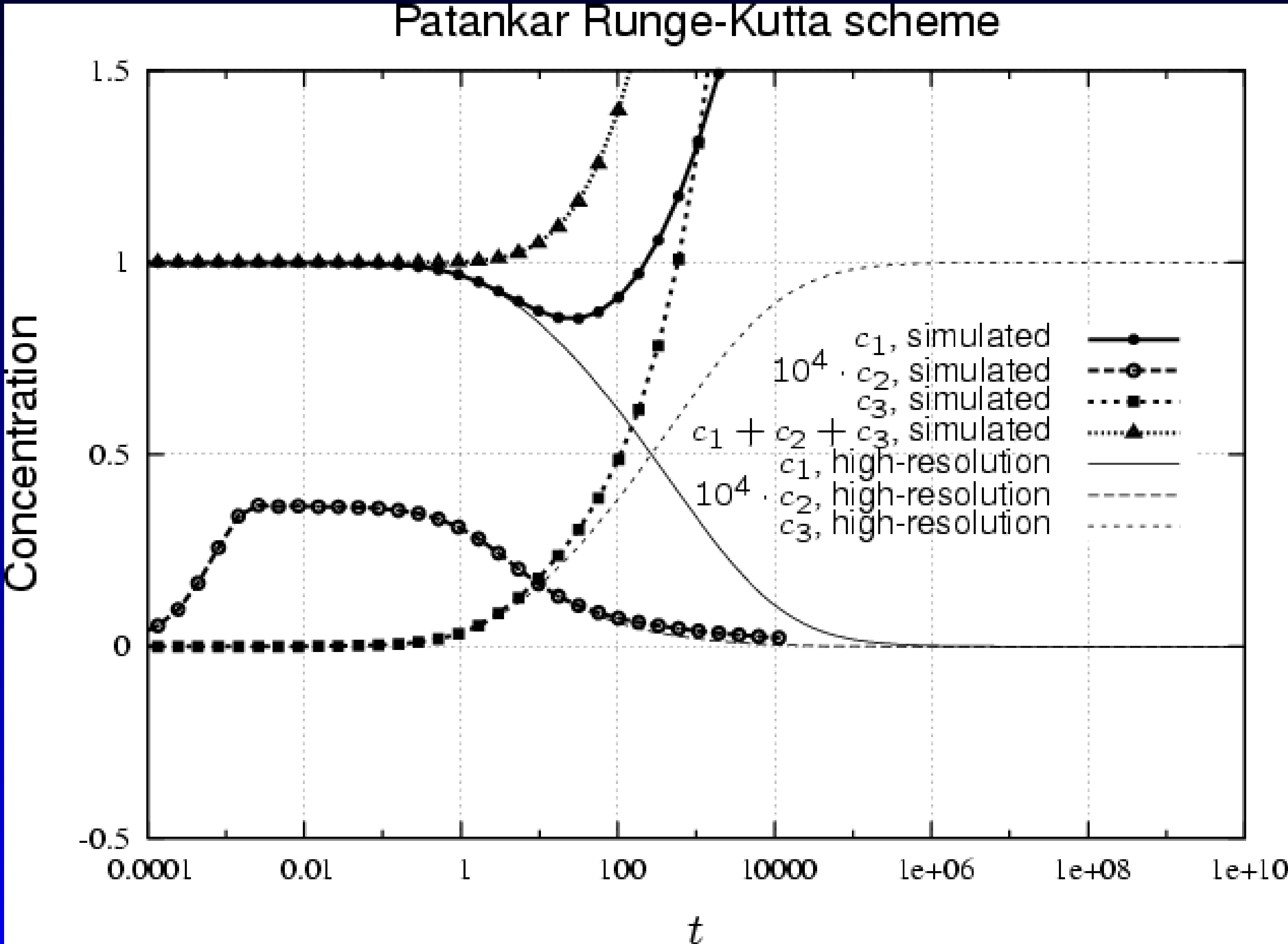
Robertson test case

$$
\begin{aligned}
d_t c_1 &= A c_2 c_3 - B c_1 \\
d_t c_2 &= B c_1 - A c_2 c_3 - C c_2^2 \\
d_t c_3 &= C c_2^2
\end{aligned}
\tag{14}
$$

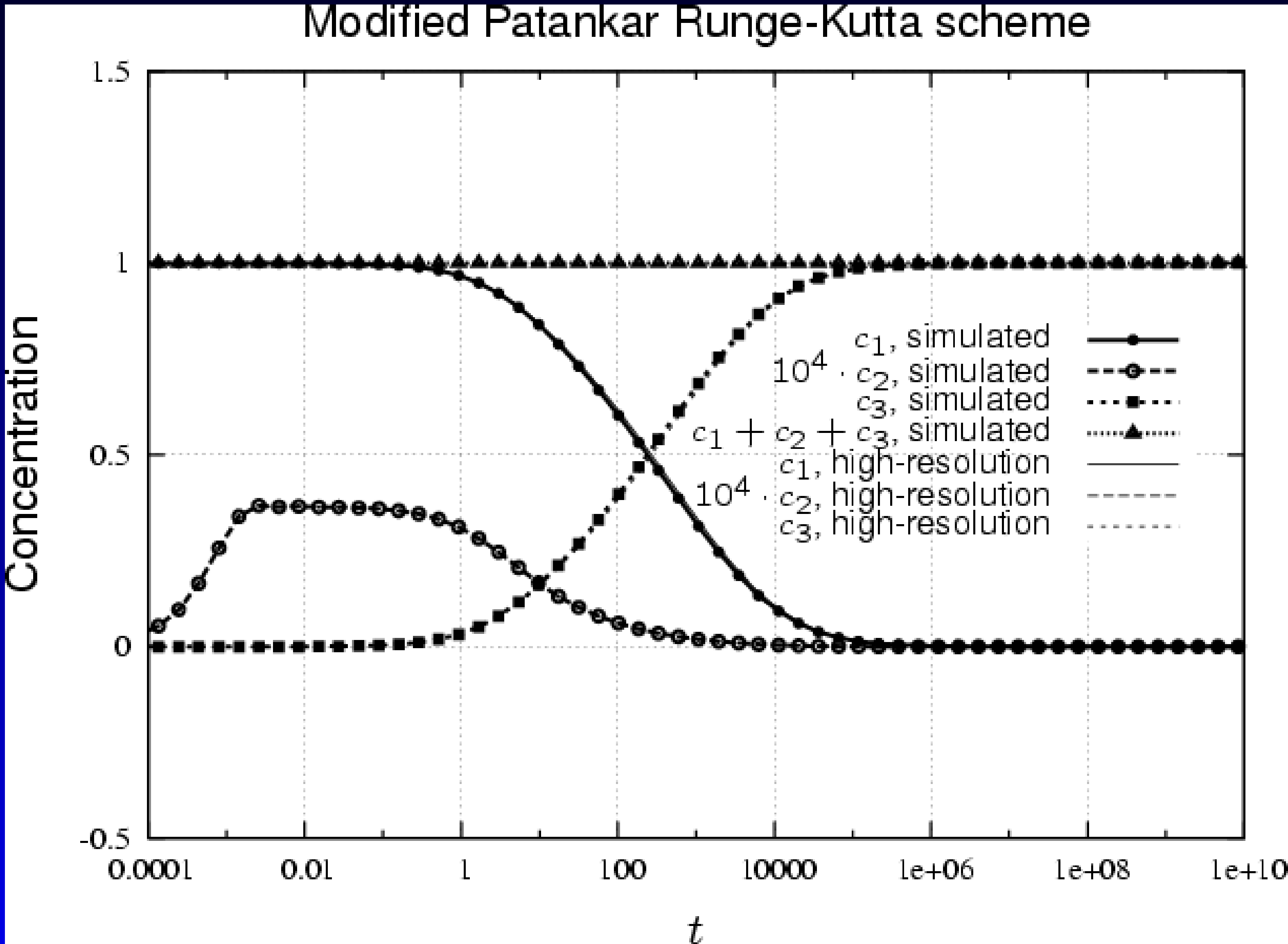
$A = 10^4$, $B = 0.04$, $C = 3 \cdot 10^7$,
$c_{10} = 1$, $c_{20} = c_{30} = 0$.

Numerical solution with $\Delta t_n = 1.8^n \times 10^{-6}$ s.

Patankar-Runge-Kutta



mod. Patankar-Runge-Kutta



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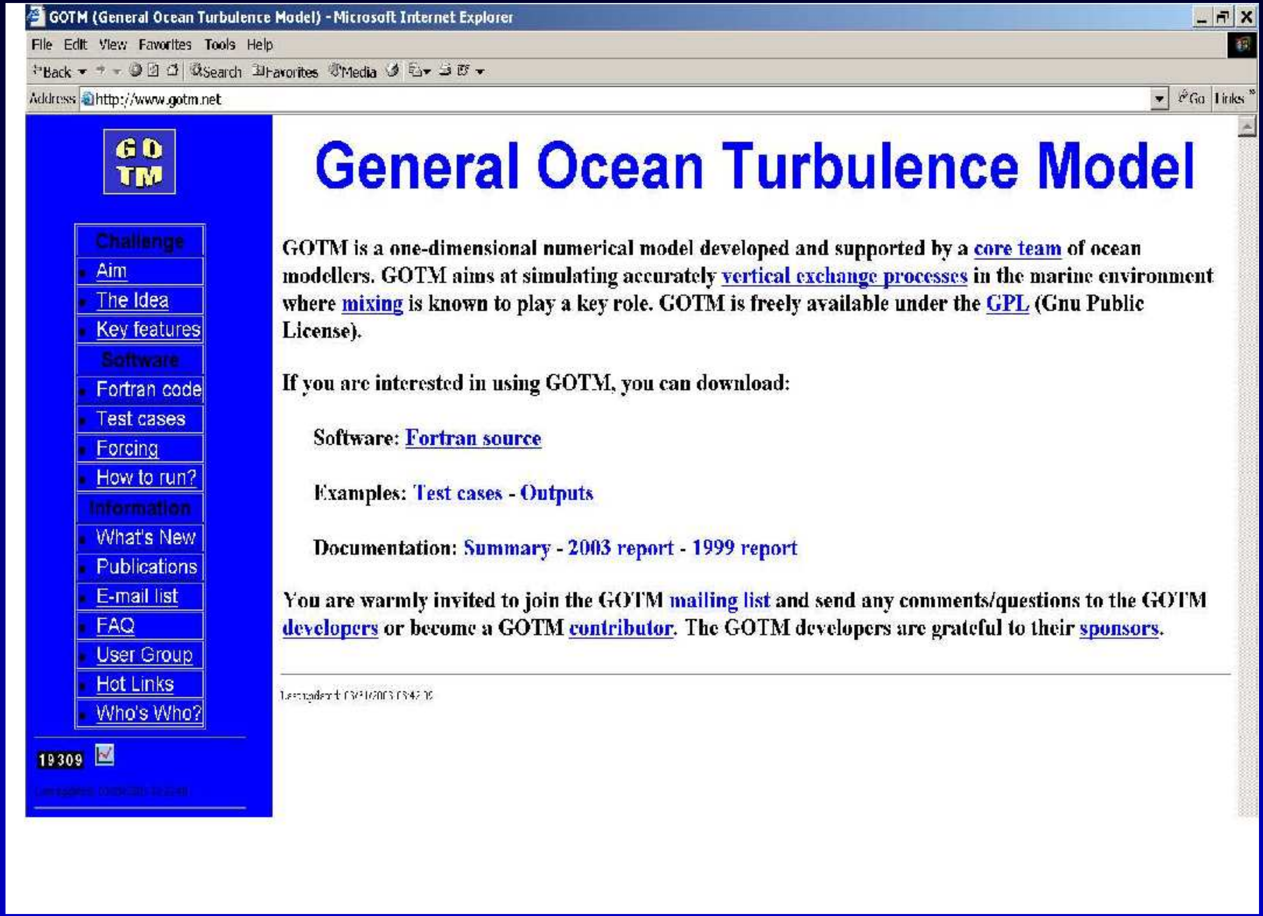
www.GOTM.net

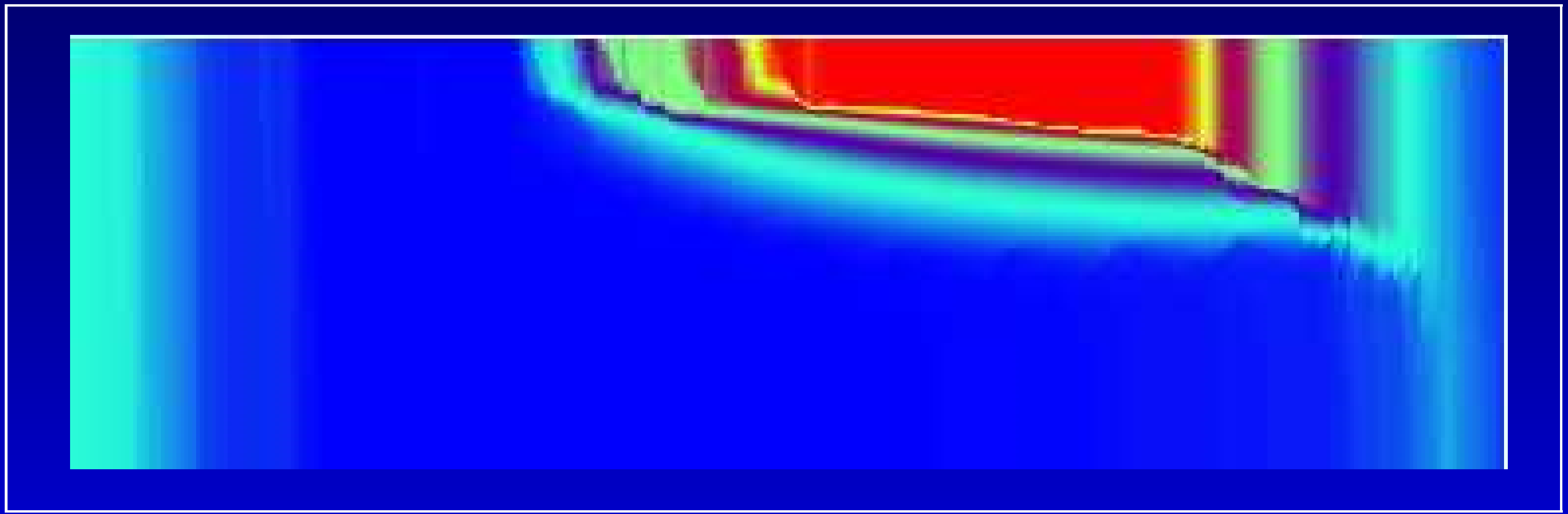


Several biogeochemical models are now implemented into GOTM.

NPZD model in GOTM

Application of GOTM with NPZD model to annual simulation of Northern North Sea.

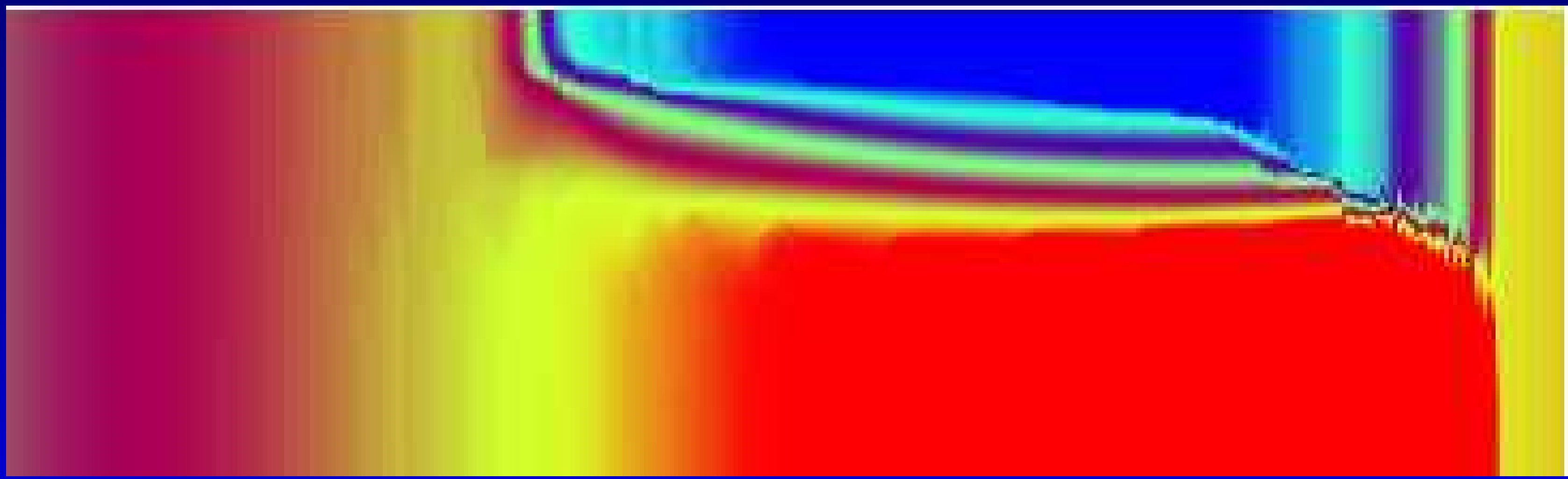
Temperature



Range: 6°C (blue) to 14°C (red). Depth: 110 m.

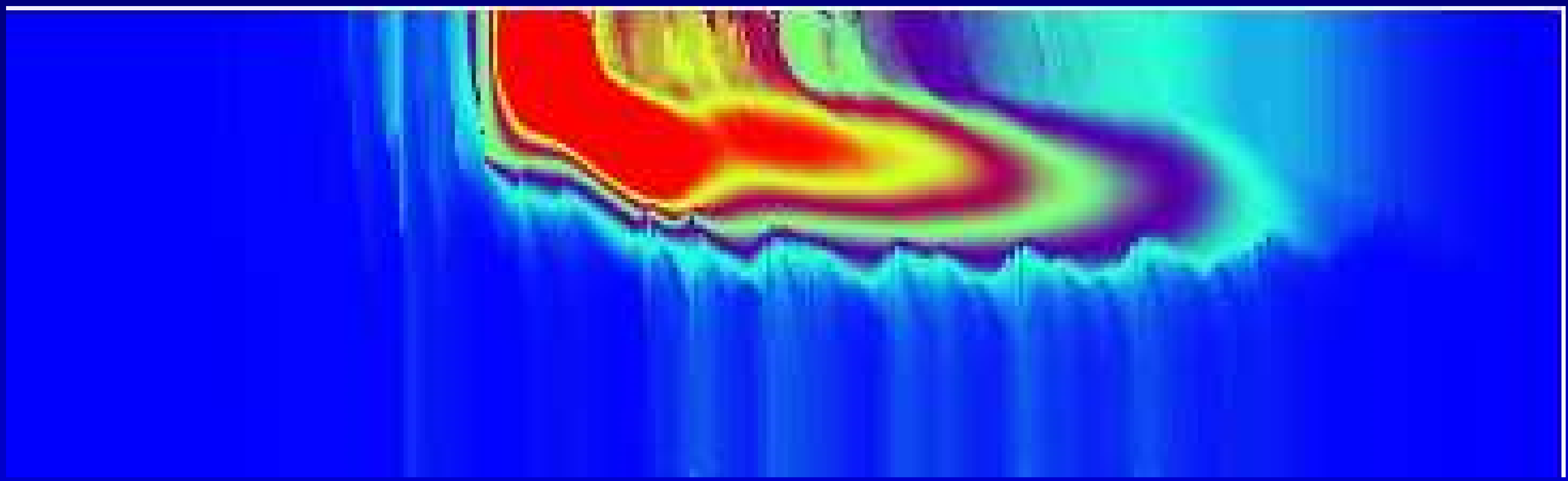
NPZD model in GOTM

Nutrients



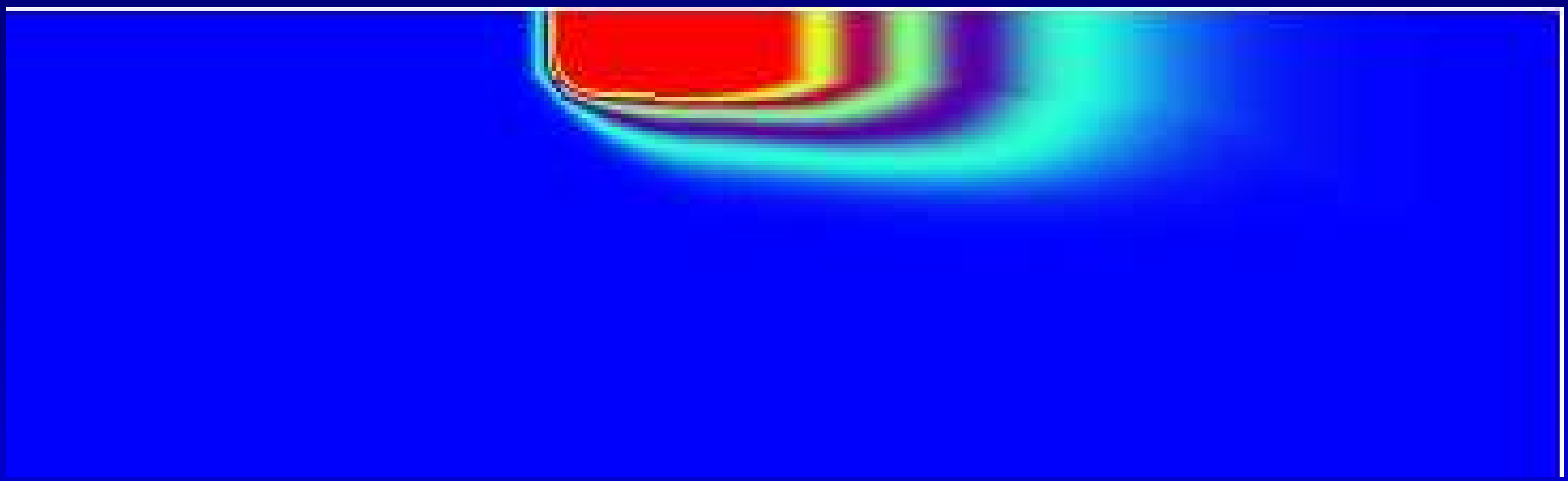
NPZD model in GOTM

Phytoplankton



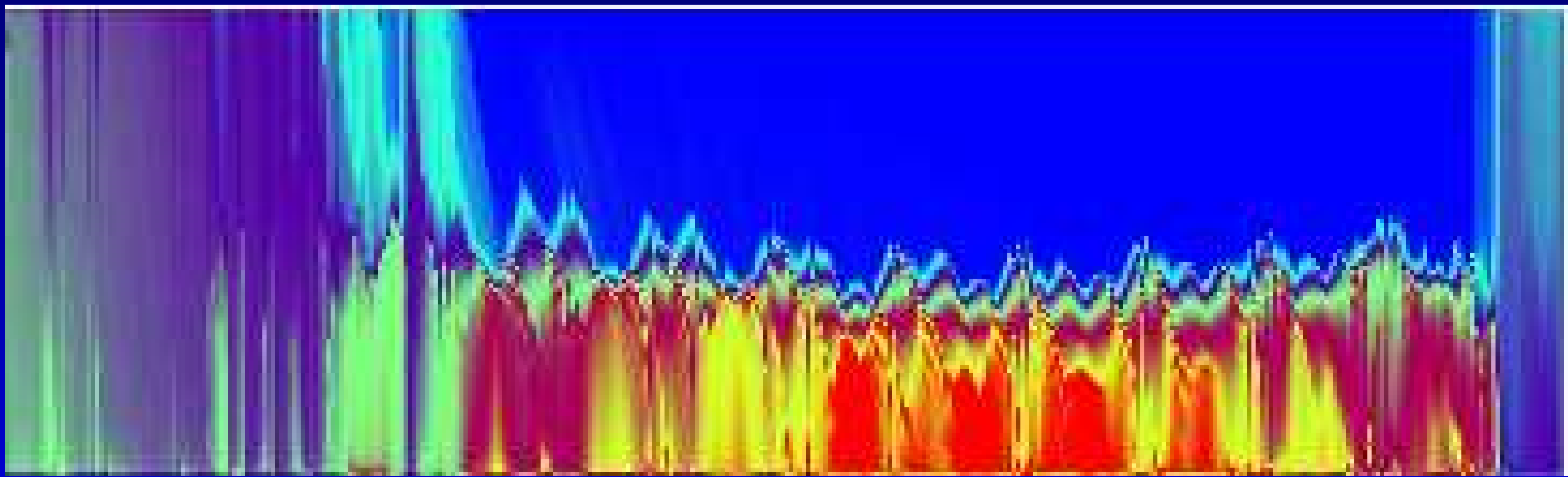
NPZD model in GOTM

Zooplankton



NPZD model in GOTM

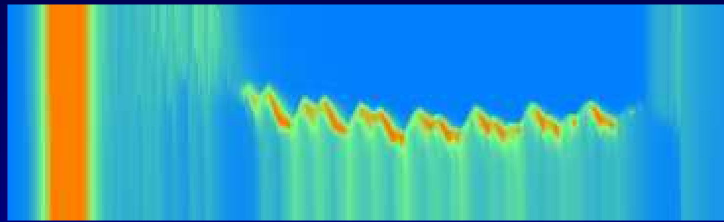
Detritus



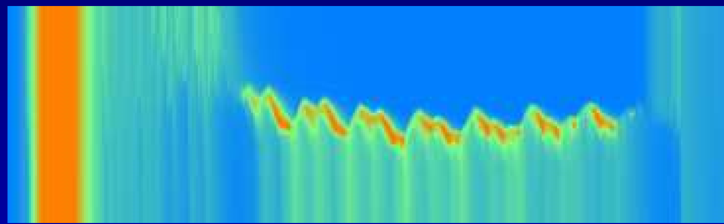
NPZD model

Phytoplankton conc. for max. nutrient uptake multiplied by a factor of 100. Short time step: $\Delta t = 1$ h, long time step: $\Delta t = 3$ h.

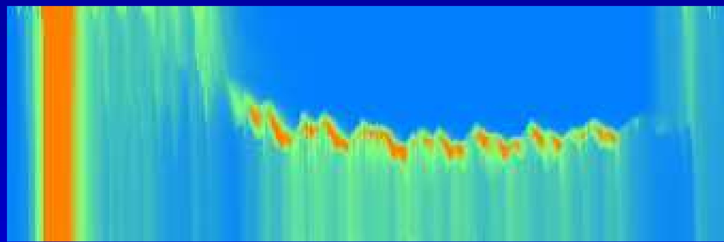
Euler, short Δt:



MPRK, short Δt:



MPRK, long Δt:



(Euler-forward with long time step is instable.)

Conclusions

- The modified Patankar-Runge-Kutta may prove to be useful for problems with time scales which are short with respect to the time step.
- Typical problems are chemical reactions in the water column and in the sediment.
- The authors of this presentation are still looking for simple and realistic test cases. Help from the JONSMOD community will be appreciated.