Why the *Euler*-scheme in particle-tracking is not enough: the shallow-sea pycnocline test case

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Outline

A simple diffusion equation

$$\partial_t C = \partial_z \left(K \partial_z C \right)$$

with

$$\begin{aligned} K &= const \\ \text{IC} &: C(0, z) = \delta(z - z_0) \end{aligned}$$

and solution

$$C(t, z) = \frac{1}{\sqrt{4\pi K t}} e^{-\frac{z^2}{4Kt}}$$

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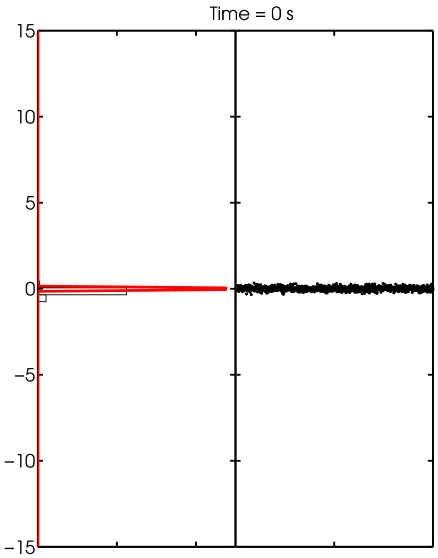

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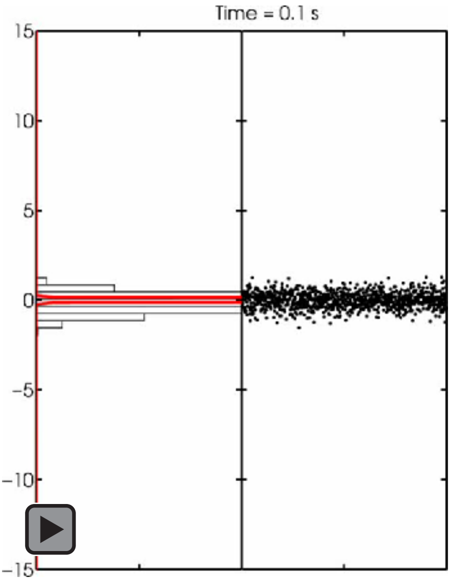


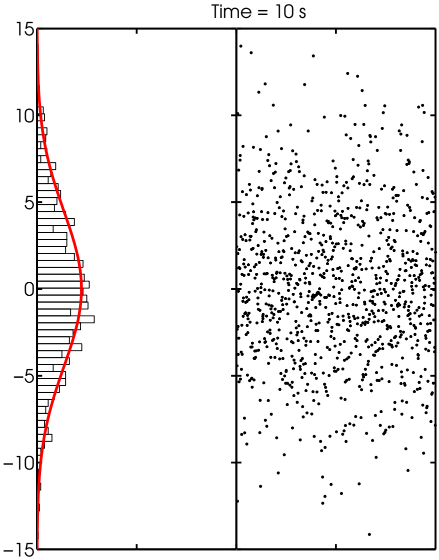
Why to use particle-tracking

Pro

- Straightforward physical interpretation
- Assessment of integrated properties (residence time, trajectories, . . .)
- Aggregation/fragmentation
- Attachment of biology/chemistry
- (No numerical diffusion)
- Inclusion of correlations or non-Gaussian statistics

Cons

- Post processing statistics
- Bin size
- Extreme values
- Computational expense



The Lagrangian framework

An advection-diffusion equation (1D)

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$$\partial_t p(z,t|t_0) = \left(w + \partial_z K(z) \right) \partial_z p \ + \ K(z) \partial_z^2 p$$

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SDE defined in the Îto sense (Arnold(1974))

$$dZ(t) = (w \ + \ \partial_z K(z))\, dt \ + \ \sqrt{2\, K(z)}\ dW(t)$$

$$\langle W(t) \rangle = 0 \ ; \ Std\, (W(t) - W(s)) = \sqrt{|t-s|}.$$

Discretisation

$$dZ(t) = a\,dt \,+\, b\,dW$$

$$\text{or} \quad Z_t = Z_0 \,+\, \int_0^t a\,ds \,+\, \int_0^t b\,dW$$

with $a = w \,+\, \partial_z K(z)$, and $b = \sqrt{2\,K(z)}$

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- Euler-scheme, (E1)

$$Z_{n+1} = Z_n + a\,\Delta t + b\,\Delta W_n$$

$$\text{with } \Delta W_n = N(0, \sqrt{\Delta t})$$

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$$\langle |Z_n - Z(\tau)| \rangle \quad \leq \quad \Lambda\,\Delta t^{\gamma} \quad : \text{strong convergence}$$

$$|\langle p(Z_n)\rangle - \langle p(Z(\tau))\rangle| \quad \leq \quad \Lambda\,\Delta t^{\gamma} \quad : \text{weak convergence}$$

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- Milstein-scheme, (M1)

$$Z_{n+1} = Z_n \;+\; a\,\Delta t \;+\; b\,\Delta W_n \;+\; \frac{1}{2} b b' \left(\Delta {W_n}^2 - \Delta t \right)$$

Discretisation

$$dZ(t) = a\,dt \;+\; b\,dW$$

- 2nd order Milstein-scheme, (M2)

$$\begin{aligned} Z_{n+1} \quad &= \quad Z_n \;+\; a\,\Delta t \;+\; b\,\Delta W_n \;+\; \frac{1}{2} b b' \left(\Delta W_n{}^2 - \Delta t \right) \;+ \\ & \frac{1}{2}\left(a a' + \frac{1}{2} a'' b^2 \right) \Delta t^2 \;+\; \frac{1}{2}\left((ab)' + \frac{1}{2} b'' b^2 \right) \Delta W_n \Delta t \end{aligned}$$

Discretisation

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- 2nd order Milstein-scheme, (M2)

$$\begin{aligned} Z_{n+1} \;=\;& Z_n \;+\; a\,\Delta t \;+\; b\,\Delta W_n \;+\; \frac{1}{2}bb'\left(\Delta W_n{}^2 - \Delta t\right) \;+ \\ & \frac{1}{2}\left(aa' + \frac{1}{2}a''b^2\right)\Delta t^2 \;+\; \frac{1}{2}\left((ab)' + \frac{1}{2}b''b^2\right)\Delta W_n \Delta t \end{aligned}$$

- 1.5 order strong Taylor-scheme, (S15)

$$\begin{aligned} Z_{n+1} \;=\;& Z_n + a\,\Delta t + b\,\Delta W_n + \frac{1}{2}bb'\left(\Delta W_n{}^2 - \Delta t\right) + a'b\Delta Z_n + \\ & \frac{1}{2}\left(aa' + \frac{1}{2}b^2a''\right)\Delta t^2 + \left(ab' + \frac{1}{2}b^2b''\right)(\Delta W_n \Delta t + \Delta Z_n) + \\ & \frac{1}{2}b\left(bb'' + (b')^2\right)\left(\frac{1}{3}\Delta W_n{}^2 - \Delta t\right)\Delta W_n \end{aligned}$$

Summary

Table: Summary of the different numerical schemes and related abbreviations. Shown are the theoretical order of convergence and the interpolation method used.

Scheme	short name	weak order	strong order	interpolation
Euler	E1	1	0.5	linear
Milstein 1st order	M1	1	1	linear
Milstein 2nd order	M2	2	1	cubic splines
Strong Taylor	S15	2	1.5	cubic splines

Motivation

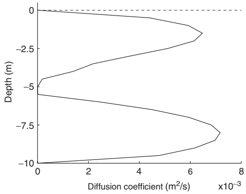

Figure 6. The vertical diffusion profile in a rectangular channel.

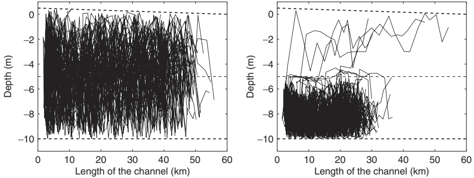

Figure 7. The release of 100 particles in stratified flow in a channel. A vertical cross section of the channel is shown. On the left side a numerical simulation with the Euler scheme, and on the right side the same simulation with the higher order stochastic Runge–Kutta scheme. The simulation time was equal to 36 h, with a time step of one hour.

Figure: Taken from: Stijnen, J. W., Heemink, A.W., and Lin, H. X.: An efficient 3D particle transport model for use in stratified flow, International Journal for Numerical Methods in Fluids 51(3), 331-350, 2006.

Motivation

$$K(z) = \overline{K}\,\frac{2(1+a)(1+2a)}{a^2 H^{1+1/a}} \begin{cases} z(H-2z)^{1/a} & , \quad 0 \le z < H/2 \\ (H-z)(2z-1)^{1/a} & , \quad H/2 \le z < H \end{cases}$$

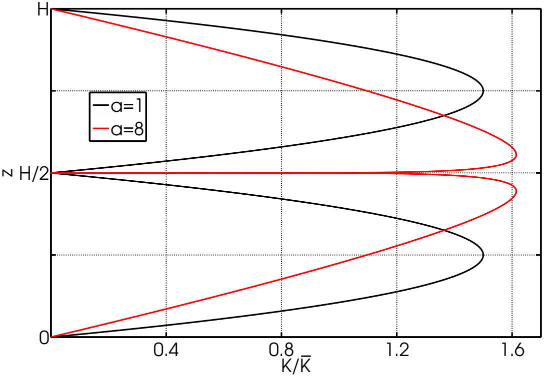

Figure: Diffusivity profile K for two different values of a.

Qualitative results

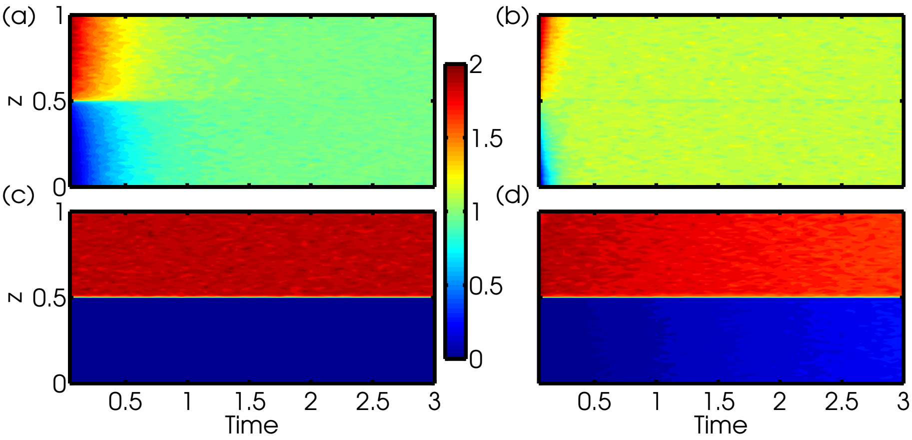

Figure: Dispersion of a particle cloud initially located at z=0.75 for two different schemes and two sets of a. Colour-coded is the particle concentration for a) *E1*-scheme with a=1, b) *E1* with a=4, c) *M2* with a=1, and d) *M2* with a=4. The time step is $\Delta t = 10^{-6}$.

Variation of the time step

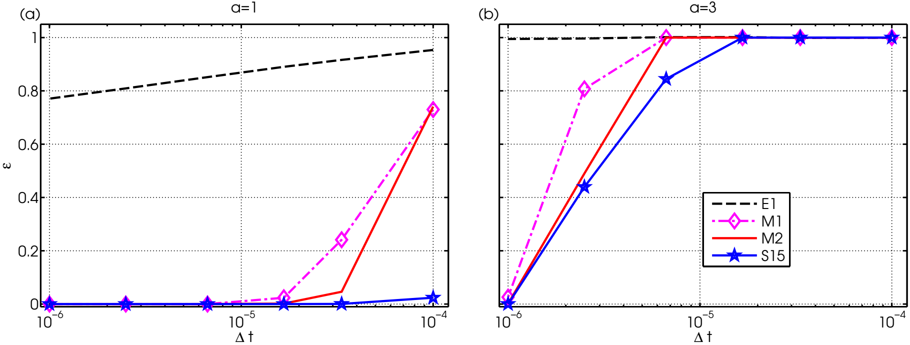

Figure: Variation of the error ε for the different numerical schemes and for a fixed parameter a with: a) a=1 and b) a=3. On the x-axis we show the time step Δt and on the y-axis the error ε.

Why the Euler-scheme fails

$$Z_{n+1} = Z_n + \partial_z K \, \Delta t + \sqrt{2K} \Delta W_n \quad : \textit{E1}\text{-scheme}$$

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- E1U-scheme

$$\Delta W_U = 2\sqrt{3} \; \left(U - \frac{1}{2} \right) \; \sqrt{\Delta t} \quad \text{with} \quad U = [0, 1]$$

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- E1T-scheme

$$P(\Delta W_T = \pm\sqrt{\Delta t}) = \frac{1}{2}$$

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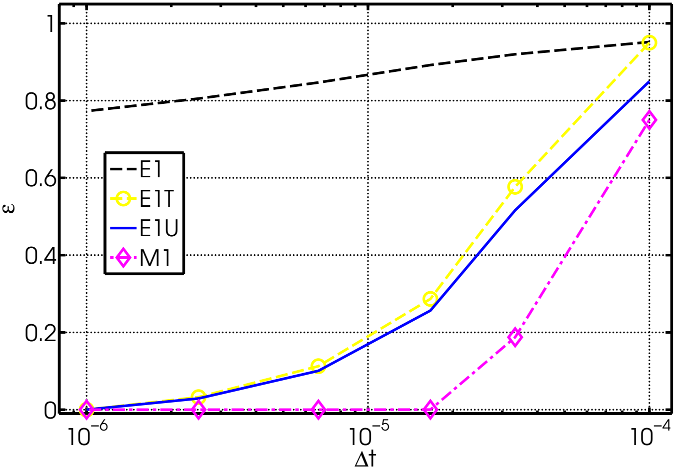

Figure: Variation of the error ε for different noise increments of the *E1*-scheme with a=1. On the y-axis the error ε is shown. As reference the *M1*-scheme is included.

Conclusions

- **Do not use the Euler-scheme in stratified environments!**

Gräwe U. (2011) Implementation of high-order particle-tracking schemes in a water column model, *Ocean Modelling* 36(1-2), 80-89

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Conclusions

- **Do not use the Euler-scheme in stratified environments!**
- The Milstein-scheme (M1) is accurate and efficient.

$$Z_{n+1} = Z_n + a\,\Delta t + b\,\Delta W_n + \frac{1}{2} bb' \left(\Delta W_n^{\,2} - \Delta t \right),$$

with $a = w + \partial_z K(z)$ and $b = \sqrt{2\,K(z)}$ $\rightarrow$ it follows that $bb' = \partial_z K(z)$

$$Z_{n+1} = Z_n + w\Delta t + \frac{1}{2}\partial_z K(\Delta W_n^{\,2} + \Delta t) + \sqrt{2\,K}\Delta W_n$$

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Timestep limitations

$$\Delta t_{max} \ll \min\left(\frac{1}{\partial_{zz} K}\right) \quad \text{(Visser(1997))}$$

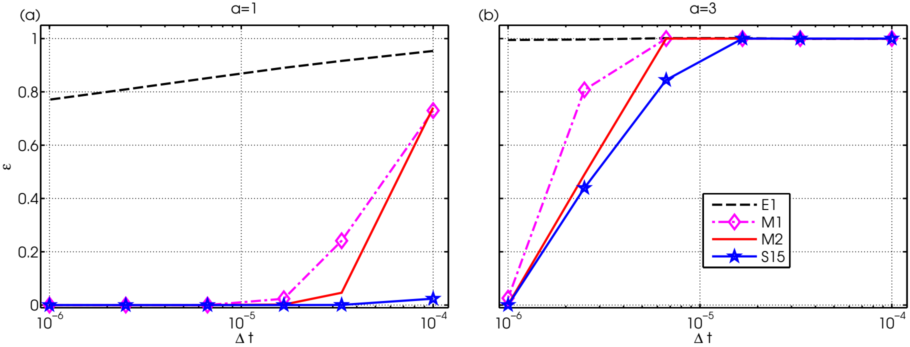
At $z = 0.5$ the curvature of the diffusivity behaves as:

$$\partial_{zz} K(z)\Big|_{z=0.5} \propto \lim_{z \to 0.5} (1 - 2z)^{\frac{1-2a}{a}}$$

Table: Time step limits for different values of a for the discretised version of the diffusivity profile.

a	1	2	4	8
Δt_{max}	$1 \cdot 10^{-3}$	$4 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$1 \cdot 10^{-4}$

Timestep limitations



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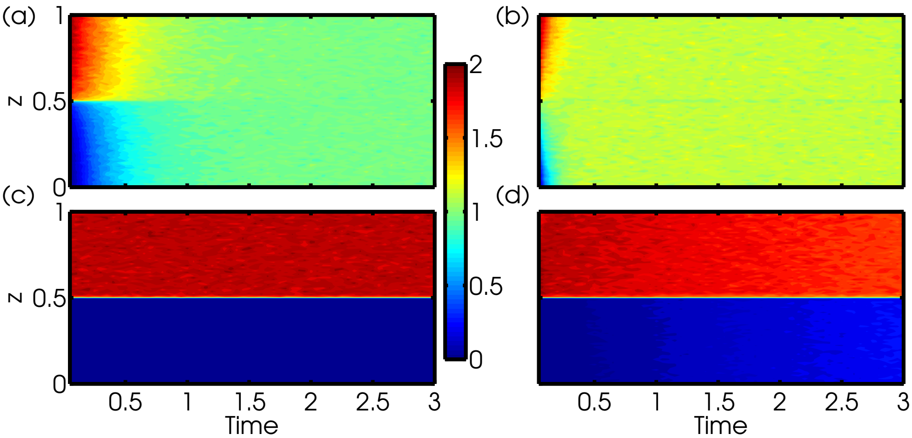
Qualitative results



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The pycnocline test case

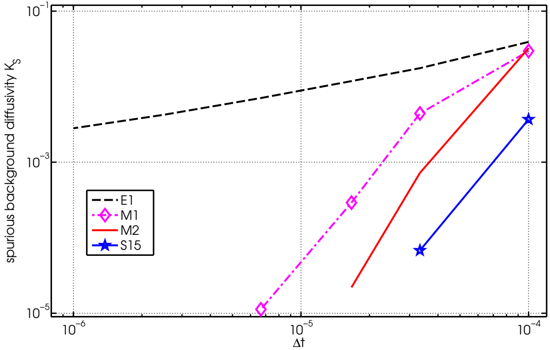

Figure: Variation of the spurious background diffusivity K_S for the different numerical schemes and for a fixed parameter a=1.

The pycnocline test case

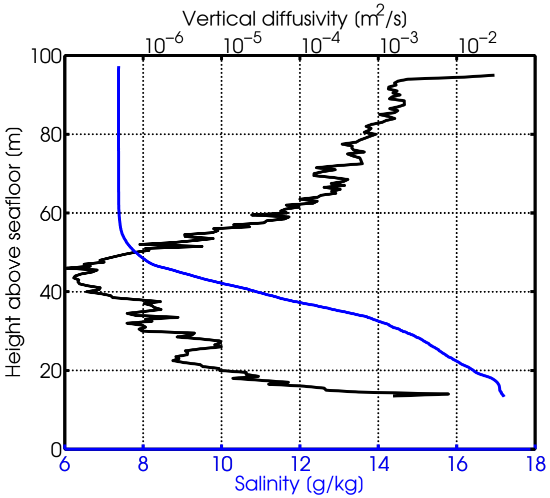

Figure: Salinity and diffusivity profile measured in the Baltic Sea (van der Lee and Umlauf(2011)).

Random numbers

1. The Mersenne Twister (Matsumoto and Nishimura(1998)) - period of 10^{6000}
2. The "Keep It Simple Stupid" generator (Marsaglia(2003)) - period of 10^{37}
3. A Tausworthe generator (L'Ecuyer(1996)) - period of 10^{26}
4. The Marsaglia-Zaman Generator (Marsaglia and Zaman(1987)) - period of 10^{43}
5. The compiler shipped generator (IFORT) (L'Ecuyer(1988)) - period of 10^{18}

The *Ziggurat* algorithm of Marsaglia and Tsang (2000) maps uniform random numbers to Gaussian ones.

Table: Comparison of time needed to generate 10^9 random numbers (in seconds). In the last row also the time is included to generate 10^9 Gaussian random numbers (based on the KISS generator).

	MT19937	KISS	Tau88	MZ144	IFORT	Ziggurat
10^9 numbers	9.63	5.88	6.08	12.82	15.85	12.91

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