

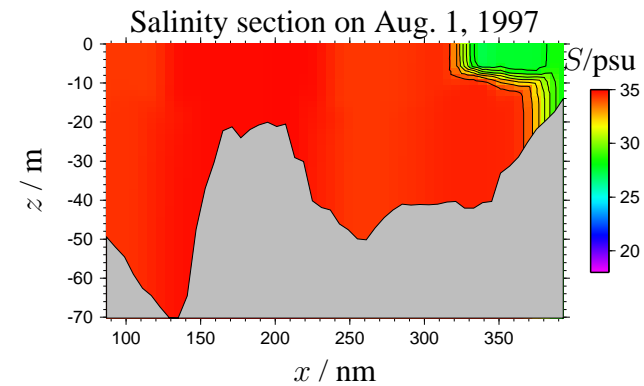
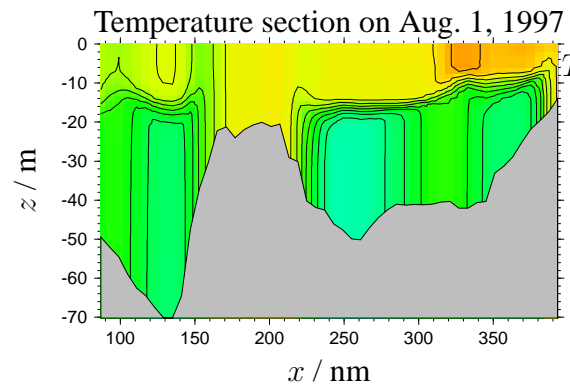
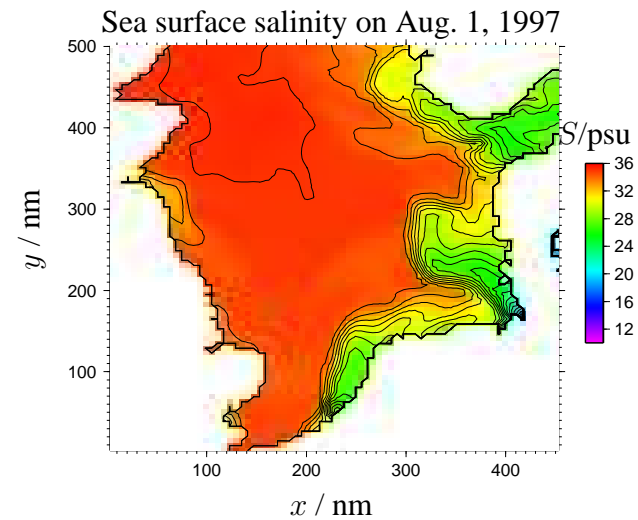
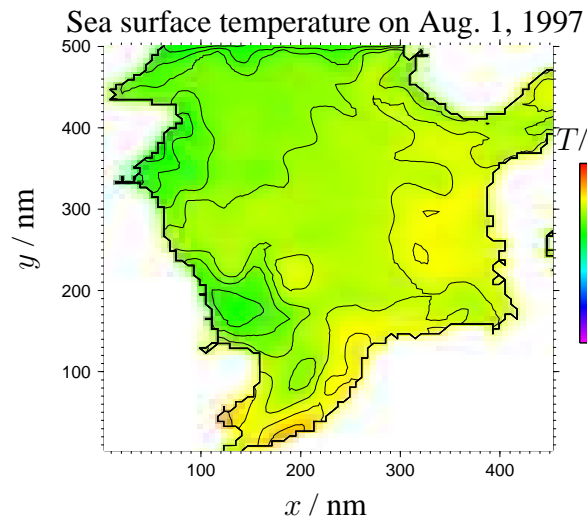
*Numerische Verfahren zur Lösung  
partieller Differentialgleichungen  
in der Physikalischen Ozeanographie*

**Hans Burchard**

<sup>1</sup>[hans.burchard@io-warnemuende.de](mailto:hans.burchard@io-warnemuende.de)

**Institut für Ostseeforschung Warnemünde**

# Nordsee-Simulation



SSS in North Sea / Baltic Sea, 1997

# $u$ -Gleichung

$$\partial_t u \quad \underbrace{+\partial_x(u^2) + \partial_y(uv) + \partial_z(uw)}_{\text{Advektion (3)}}$$

$$-\partial_z((\nu_t + \nu)\partial_z u) - \partial_x(2A_h^M \partial_x u) - \partial_y(A_h^M(\partial_y u + \partial_x v))$$

$$-fv \quad \underbrace{-\int_z^\zeta \partial_x b \, dz'}_{\text{Druckgradient (1)}} = -\partial_x \left( g\zeta + \frac{1}{\rho_0} p_0 \right).$$

(1)

$$b = -g \frac{\rho - \rho_0}{\rho_0} \quad (2)$$

# v-Gleichung

$$\partial_t v \quad \underbrace{+\partial_x(vu) + \partial_y(v^2) + \partial_z(vw)}_{\text{Advektion (3)}}$$

$$-\partial_z ((\nu_t + \nu)\partial_z v) - \partial_y (2A_h^M \partial_y v) - \partial_x (A_h^M (\partial_y u + \partial_x v))$$

$$+fu \quad \underbrace{- \int_z^\zeta \partial_y b dz'}_{\text{Druckgradient (1)}} = -\partial_y \left( g\zeta + \frac{1}{\rho_0} p_0 \right).$$

(3)

# Kontinuitätsgleichung

Kontinuität:

$$\partial_x u + \partial_y v + \partial_z w = 0. \quad (4)$$

Freie Oberfläche:

$$\underbrace{\partial_t \zeta = -\partial_x U - \partial_y V.}_{\text{mode splitting (2)}} \quad (5)$$

mit

$$U = \int_{-H}^{\zeta} u \, dz, \quad V = \int_{-H}^{\zeta} v \, dz. \quad (6)$$

# Tracer-Gleichung

$$\partial_t c^i \quad \underbrace{+\partial_x(uc^i) + \partial_y(vc^i) + \partial_z((w + w_s^i)c^i)}_{\text{Advektion (3)}} - \partial_z(\nu'_t \partial_z c^i)$$

$$-\partial_x(A_h^T \partial_x c^i) - \partial_y(A_h^T \partial_y c^i) = \underbrace{\sum_{j=1}^N (p_{ij} - d_{ij})}_{\text{mod. Patankar (6)}} \quad (7)$$

$$\rho = \rho(c^1, c^2, \dots, c^N, p_0) \quad (8)$$

# Turbulenz-Modell

$$\partial_t k - \partial_z \left( \left( \nu + \frac{\nu_t}{\sigma_k} \right) \partial_z k \right) = P + B \quad \underbrace{-\varepsilon}_{\text{Patankar (5)}}, \quad (9)$$

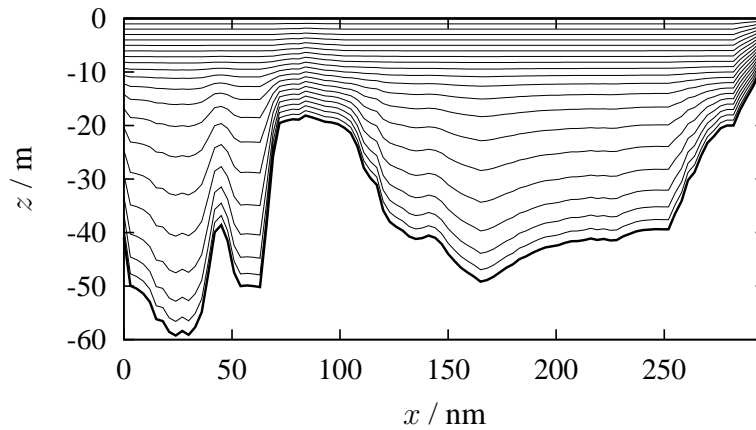
$$\partial_t \varepsilon - \partial_z \left( \left( \nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \partial_z \varepsilon \right) = \frac{\varepsilon}{k} (c_1 P + c_3 B \quad \underbrace{-c_2 \varepsilon}_{\text{Patankar (5)}}), \quad (10)$$

$$P = \nu_t \underbrace{\left( (\partial_z u)^2 + (\partial_z v)^2 \right)}_{\text{Energieerhaltung (4)}}, \quad B = -\nu_t' \partial_z b, \quad (11)$$

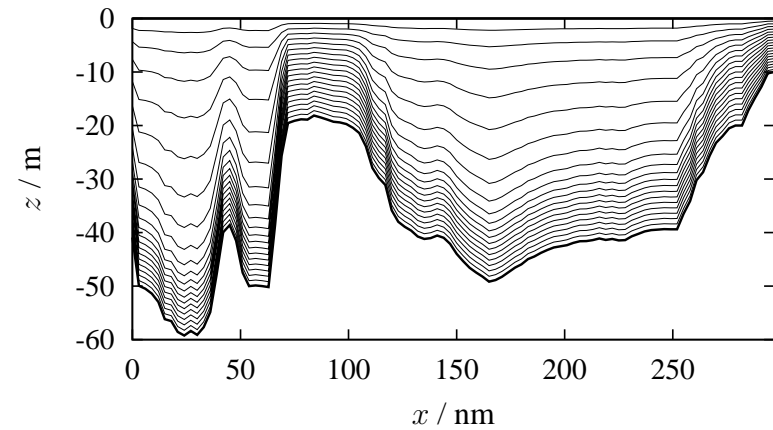
$$\nu_t = c_\mu \frac{k^2}{\varepsilon}, \quad \nu_t' = c_\mu' \frac{k^2}{\varepsilon}. \quad (12)$$

# Vertikale Koordinaten

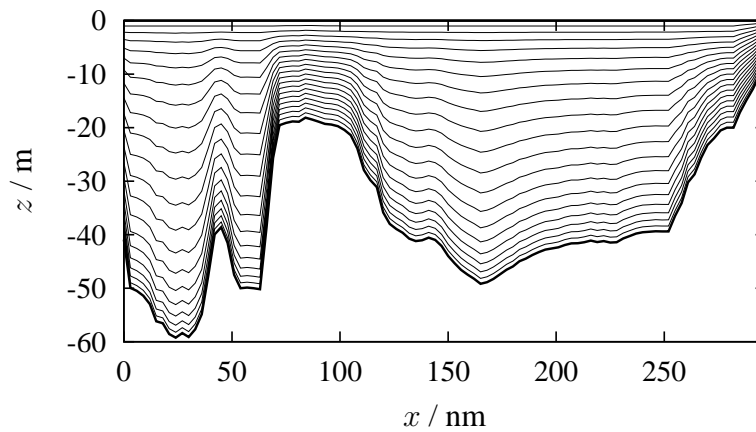
upper  $\gamma$ -coordinates,  $d_u = 5, d_l = 1.5$



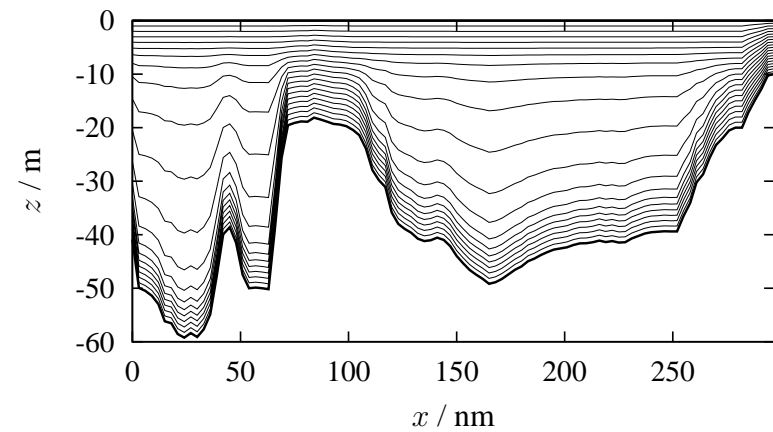
lower  $\gamma$ -coordinates,  $d_u = 1.5, d_l = 5$



symmetric  $\gamma$ -coordinates,  $d_u = 1.5, d_l = 1.5$



symmetric  $\gamma$ -coordinates,  $d_u = 5, d_l = 5$



# Schichtgemittelte Gleichungen

$$\partial_t p_k + \partial_x(u_k p_k) + \partial_y(v_k p_k) + \bar{w}_k \tilde{u}_k - \bar{w}_{k-1} \tilde{u}_{k-1} - \tau_k^x + \tau_{k-1}^x$$

$$- \partial_x (2A_k^M h_k \partial_x u_k) - \partial_y (A_k^M h_k (\partial_y u_k + \partial_x v_k)) - f q_k$$

$$- h_k \left( \frac{1}{2} h_N (\partial_x^* b)_N + \sum_{j=k}^{N-1} \frac{1}{2} (h_j + h_{j+1}) (\partial_x^* b)_j \right) = -g h_k \partial_x \zeta, \quad (13)$$

$$p_k := \int_{z_{k-1}}^{z_k} u \, dz, \quad q_k := \int_{z_{k-1}}^{z_k} v \, dz, \quad (14)$$

# Dichtegradient, diskret

$$\begin{aligned}(\partial_x^* b)_k &= \frac{1}{2}(\partial_x b_{k+1} + \partial_x b_k) - \partial_x z_k \frac{b_{k+1} - b_k}{\frac{1}{2}(h_{k+1} + h_k)} \\ &\sim \frac{\frac{1}{2}(b_{i+1,k+1} + b_{i+1,k}) - \frac{1}{2}(b_{i,k+1} + b_{i,k})}{\Delta x} \\ &\quad - \partial_x z_k \frac{\frac{1}{2}(b_{i+1,k+1} + b_{i,k+1}) - \frac{1}{2}(b_{i+1,k} + b_{i,k})}{\frac{1}{2}(h_{i,k}^c + h_{i+1,k}^c)}\end{aligned}\tag{15}$$

# Hydrostatische Konsistenz

$$(\partial_x^* b)_k \sim \frac{(\frac{1}{2} + \alpha)b_{i+1,k+1} + (\frac{1}{2} - \alpha)b_{i+1,k}}{\Delta x} \quad (16)$$

$$\frac{(\frac{1}{2} + \alpha)b_{i,k+1} + (\frac{1}{2} - \alpha)b_{i,k}}{\Delta x}$$

$$\alpha = \frac{\partial_x z_k \Delta x}{h_{i,k}^c + h_{i+1,k}^c}. \quad (17)$$

Hydrostatische Konsistenzbedingung:

$$|\partial_x z_k| \frac{\Delta x}{\frac{1}{2}(h_{i,k}^c + h_{i+1,k}^c)} \leq 1. \quad (18)$$

# Lösungsstrategien

- Hohe horizontale Auflösung
- Geringe vertikale Auflösung
- Geringe Neigung der Koordinaten
- Verfahren höherer Ordnung
- Interpolation in  $z$ -Koordinaten
- Monotone Verfahren

# Mode splitting

## Problem:

Barotropes Zeitschrittkriterium:

$$\Delta t < \left[ \frac{1}{2} \left( \frac{1}{\Delta x} + \frac{1}{\Delta y} \right) \sqrt{2gD} \right]^{-1}. \quad (19)$$

Baroklines Zeitschrittkriterium:

$$\Delta t < \min \left\{ \frac{\Delta x}{u_{\max}}, \frac{\Delta y}{v_{\max}} \right\}. \quad (20)$$

# Lösungsstrategie

Vertikal-integrierte Gleichung:

$$\partial_t U + \int_{-H}^{\zeta} \partial_x u^2 dz = 0, \quad (21)$$

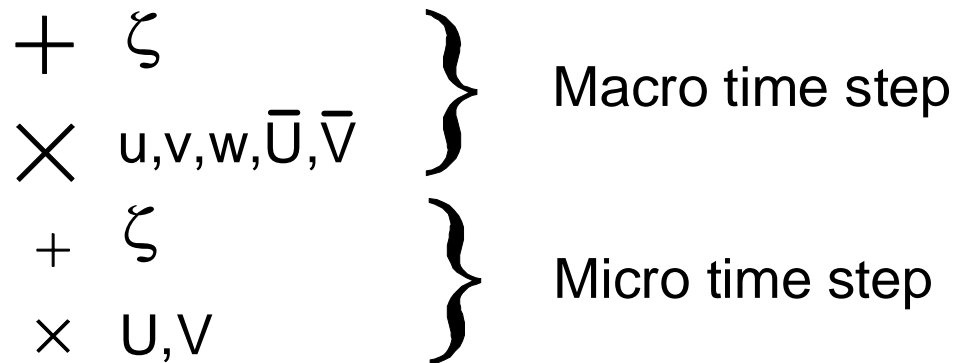
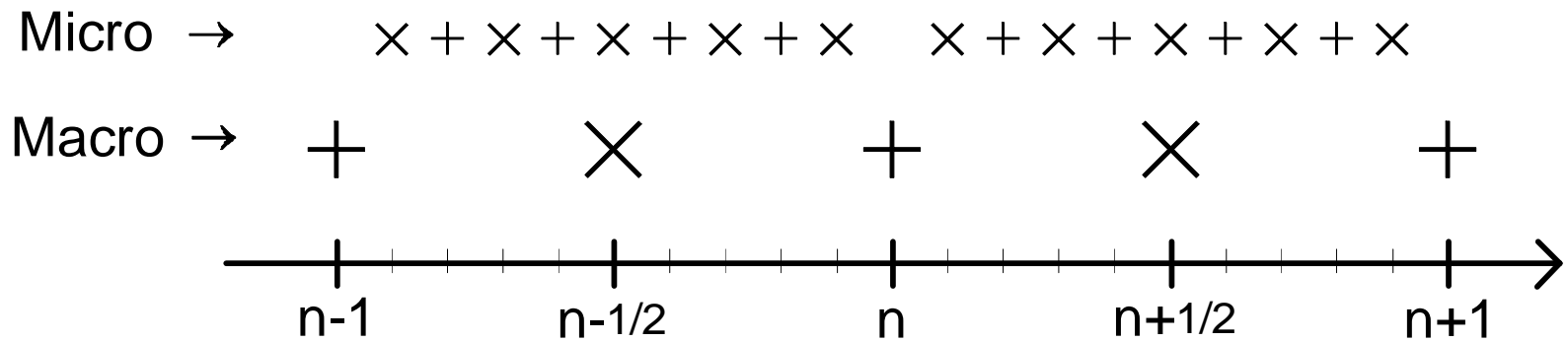
Umformung:

$$\partial_t U + \partial_x \left( \frac{U^2}{D} \right) + S_A^x = 0, \quad (22)$$

Interaktionsterm:

$$S_A^x = \int_{-H}^{\zeta} \partial_x u^2 dz - \partial_x \left( \frac{U^2}{D} \right), \quad (23)$$

# Zeitschrittschema



# TVD advection schemes I

One-dimensional linear tracer equation:

$$\partial_t \Psi + \partial_x (u \Psi) = 0 \quad (24)$$

Discretisation:

$$\Psi_i^{n+1} = \Psi_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n) \quad (25)$$

Upstream-biased flux calculation:

$$F_{i+1/2}^n = \frac{1}{\Delta t} \int_{x_{i+1/2} - u \Delta t}^{x_{i+1/2}} \Psi(x') dx'. \quad (26)$$

# TVD advection schemes II

Polynomial tracer approximation:

$$\int_{x_{i-1/2+k}}^{x_{i+1/2+k}} \tilde{\Psi}_i(x') dx' = \Psi_{i+k}, \quad k = -1, 0, 1, \quad (27)$$

Lax-Wendroff form:

$$F_{i+1/2} = \begin{cases} u_{i+1/2} \left( \Psi_i + \frac{1}{2} \Phi_{i+1/2}^+ (1 - |c_{i+1/2}|) (\Psi_{i+1} - \Psi_i) \right) & \text{for } u_{i+1/2} > 0, \\ u_{i+1/2} \left( \Psi_{i+1} + \frac{1}{2} \Phi_{i+1/2}^- (1 - |c_{i+1/2}|) (\Psi_i - \Psi_{i+1}) \right) & \text{else,} \end{cases} \quad (28)$$

$$\Phi_{i+1/2}^+ = \alpha_{i+1/2} + \beta_{i+1/2} r_{i+1/2}^+, \quad \Phi_{i+1/2}^- = \alpha_{i+1/2} + \beta_{i+1/2} r_{i+1/2}^-, \quad (29)$$

$$\alpha_{i+1/2} = \frac{1}{2} + \frac{1}{6} (1 - 2|c_{i+1/2}|), \quad \beta_{i+1/2} = \frac{1}{2} - \frac{1}{6} (1 - 2|c_{i+1/2}|), \quad (30)$$

$$r_{i+1/2}^+ = \frac{\Psi_i - \Psi_{i-1}}{\Psi_{i+1} - \Psi_i}, \quad r_{i+1/2}^- = \frac{\Psi_{i+2} - \Psi_{i+1}}{\Psi_{i+1} - \Psi_i}. \quad (31)$$

# TVD advection schemes III

P<sub>2</sub>-PDM, ULTIMATE QUICKEST (Leonard [1979]):

$$\Phi_{i+1/2}^+ \rightarrow \max \left[ 0, \min \left( \Phi_{i+1/2}^+, \frac{2}{1 - |c_{i+1/2}|}, \frac{2r_{i+1/2}^+}{|c_{i+1/2}|} \right) \right], \quad (32)$$

MUSCL (van Leer [1979]):

$$\Phi_{i+1/2}^+ \rightarrow \max \left[ 0, \min \left( 2, 2r_{i+1/2}^+, \frac{1 + r_{i+1/2}^+}{2} \right) \right], \quad (33)$$

Superbee (Roe [1985]):

$$\Phi_{i+1/2}^+ \rightarrow \max \left[ 0, \min(1, 2r_{i+1/2}^+), \min(r_{i+1/2}^+, 2) \right]. \quad (34)$$

# Directional split schemes

$$\partial_t(D\Psi) + \partial_x(uD\Psi) + \partial_y(vD\Psi) = 0 \quad (35)$$

$$\partial_t D + \partial_x(uD) + \partial_y(vD) = 0 \quad (36)$$

Directional split (Pietrzak [1998])

$$D_{i,j}^{n+1/2} \Psi_{i,j}^{n+1/2} = D_{i,j}^n \Psi_{i,j}^n - \frac{\Delta t}{\Delta x} (D_{i+1/2,j}^n F_{i+1/2,j}^n - D_{i-1/2,j}^n F_{i-1/2,j}^n) \quad (37)$$

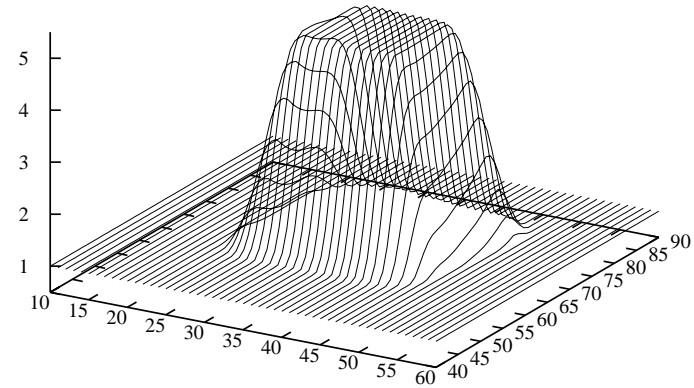
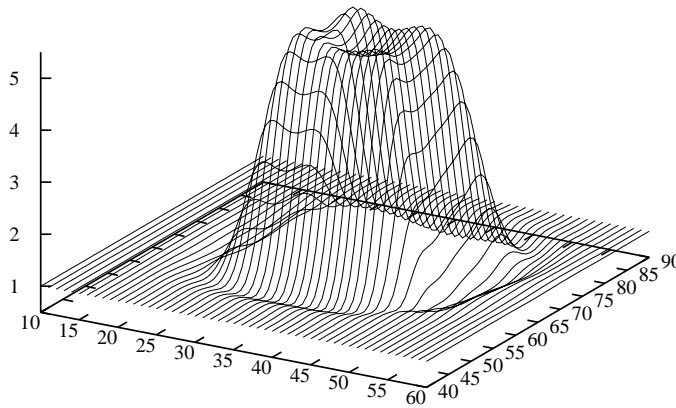
$$D_{i,j}^{n+1} \Psi_{i,j}^{n+1} = D_{i,j}^{n+1/2} \Psi_{i,j}^{n+1/2} - \frac{\Delta t}{\Delta y} (D_{i,j+1/2}^n F_{i,j+1/2}^n - D_{i,j-1/2}^n F_{i,j-1/2}^n) \quad (38)$$

$$D_{i,j}^{n+1/2} = D_{i,j}^n - \frac{\Delta t}{\Delta x} (U_{i+1/2,j}^n - U_{i-1/2,j}^n) \quad (39)$$

$$D_{i,j}^{n+1} = D_{i,j}^{n+1/2} - \frac{\Delta t}{\Delta y} (V_{i,j+1/2}^n - V_{i,j-1/2}^n). \quad (40)$$

# 2D test case: $P_2$ split scheme

Cube resulting after one solid-body rotation with  $\Delta x = \Delta y = 1$  m and a Courant number of  $c = 0.5$ .  
Left: unlimited  $P_2$  scheme; right: limited  $P_2$ -PDM scheme



# Energieerhaltung

Analytisch:

$$\partial_t \bar{u} - \partial_z (\nu_t \partial_z \bar{u}) = 0, \quad (41)$$

Diskret (Crank-Nicolson):

$$\frac{\hat{u}_j - u_j}{\Delta t} - \frac{\nu_{j+\frac{1}{2}} \frac{\bar{u}_{j+1} - \bar{u}_j}{z_{j+1} - z_j} - \nu_{j-\frac{1}{2}} \frac{\bar{u}_j - \bar{u}_{j-1}}{z_j - z_{j-1}}}{z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}}} = 0 \quad (42)$$

$$\bar{u} = \sigma \hat{u} + (1 - \sigma)u. \quad (43)$$

# Energieerhaltung

Kinetische Energie  $e_{kin} = \bar{u}^2/2$ :

$$\partial_t e_{kin} - \partial_z(\nu_t \partial_z e_{kin}) = -\nu_t (\partial_z \bar{u})^2 = -P \quad (44)$$

Diskret:

$$\begin{aligned} \frac{\hat{e}_j - e_j}{\Delta t} &= \frac{\nu_{j+1/2} \frac{\bar{e}_{j+1} - \bar{e}_j}{z_{j+1} - z_j} - \nu_{j-1/2} \frac{\bar{e}_j - \bar{e}_{j-1}}{z_j - z_{j-1}}}{z_{j+1/2} - z_{j-1/2}} = \\ &= -\frac{1}{2} \nu_{j+1/2} \frac{\sigma(\hat{u}_{j+1} - \hat{u}_j)(\hat{u}_{j+1} - u_j) + (1 - \sigma)(u_{j+1} - u_j)(u_{j+1} - \hat{u}_j)}{(z_{j+1/2} - z_{j-1/2})(z_{j+1} - z_j)} \\ &\quad - \frac{1}{2} \nu_{j-1/2} \frac{\sigma(\hat{u}_j - \hat{u}_{j-1})(\hat{u}_j - u_{j-1}) + (1 - \sigma)(u_j - u_{j-1})(\hat{u}_j - u_{j-1})}{(z_{j+1/2} - z_{j-1/2})(z_j - z_{j-1})} \\ &=: -P_{j+1/2}^l - P_{j-1/2}^u. \end{aligned}$$

# Energieerhaltung

Turbulenzproduktion, neu:

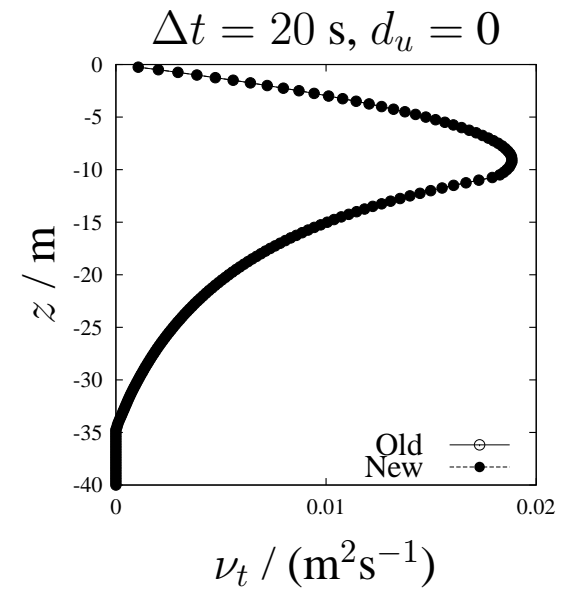
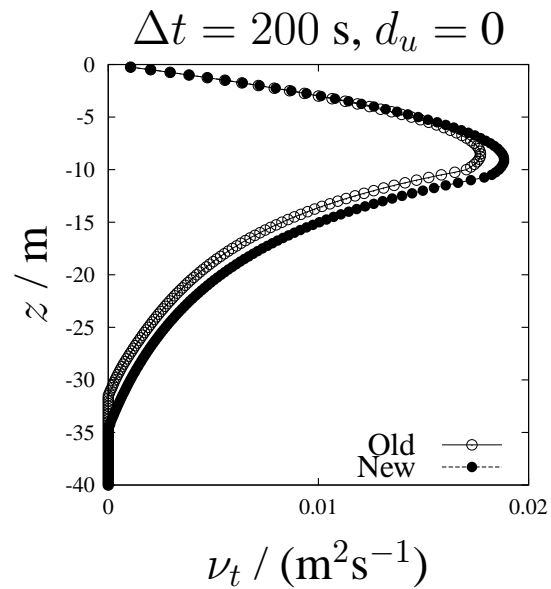
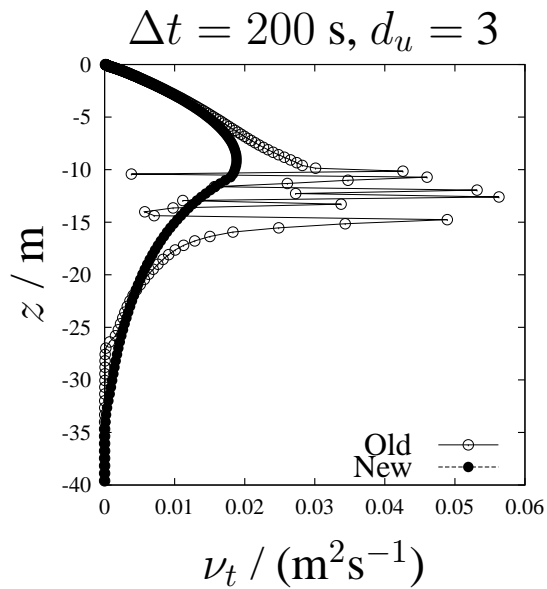
$$P_{j+1/2} = \nu_{j+1/2} \frac{(\bar{u}_{j+1} - \bar{u}_j)(\tilde{u}_{j+1} - \tilde{u}_j)}{(z_{j+1} - z_j)^2}, \quad (46)$$

$$\tilde{u}_j = \frac{1}{2}(\hat{u}_j + u_j).$$

Turbulenzproduktion, alt:

$$P_{j+1/2} = \nu_{j+\frac{1}{2}} \left[ \frac{\hat{u}_{j+1} - \hat{u}_j}{z_{j+1} - z_j} \right]^2. \quad (47)$$

# Energieerhaltung



# Patankar-Trick

$$\partial_t X = P - QX, \quad P, Q > 0 \quad (48)$$

$$\frac{X^{n+1} - X^n}{\Delta t} = P^n - Q^n X^n \quad (49)$$

$$X_i^{n+1} = X_i^n (1 - \Delta t Q_i^n) + \Delta t P_i^n, \quad (50)$$

$$\frac{X^{n+1} - X^n}{\Delta t} = P^n - Q^n X^{n+1}, \quad (51)$$

$$X^{n+1} = \frac{X^n + \Delta t P^n}{1 + \Delta t Q^n}, \quad (52)$$

# mod. Patankar-Trick

Test-Problem:

$$d_t c_i = P_i(\vec{c}) - D_i(\vec{c}) \quad , i = 1, \dots, I, \quad (53)$$

$$\vec{c}^0 = \vec{c}(t = 0) > \vec{0}, \quad (54)$$

$$P_i(\vec{c}) = \sum_{j=1}^I p_{i,j}(\vec{c}), \quad D_i(\vec{c}) = \sum_{j=1}^I d_{i,j}(\vec{c}), \quad (55)$$

$$p_{i,j}(\vec{c}) = d_{j,i}(\vec{c}), \quad \text{for } i \neq j. \quad (56)$$

# mod. Patankar-Trick

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

(57)

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

Das Gleichungssystem ist also **konservativ** für  $p_{i,i} = d_{i,i} = 0$ .

# mod. Patankar-Trick

Diskretisierungsprobleme:

- Explizite Verfahren sind nicht unbedingt nicht-negativ.
- Patankar-Verfahren sind nicht konservativ.

Problem: Suche konservatives und nicht-negatives Verfahren.

# mod. Patankar-Trick

Lösung, z.B. erster Ordnung:

modifiziertes Patankar-Euler-Verfahren:

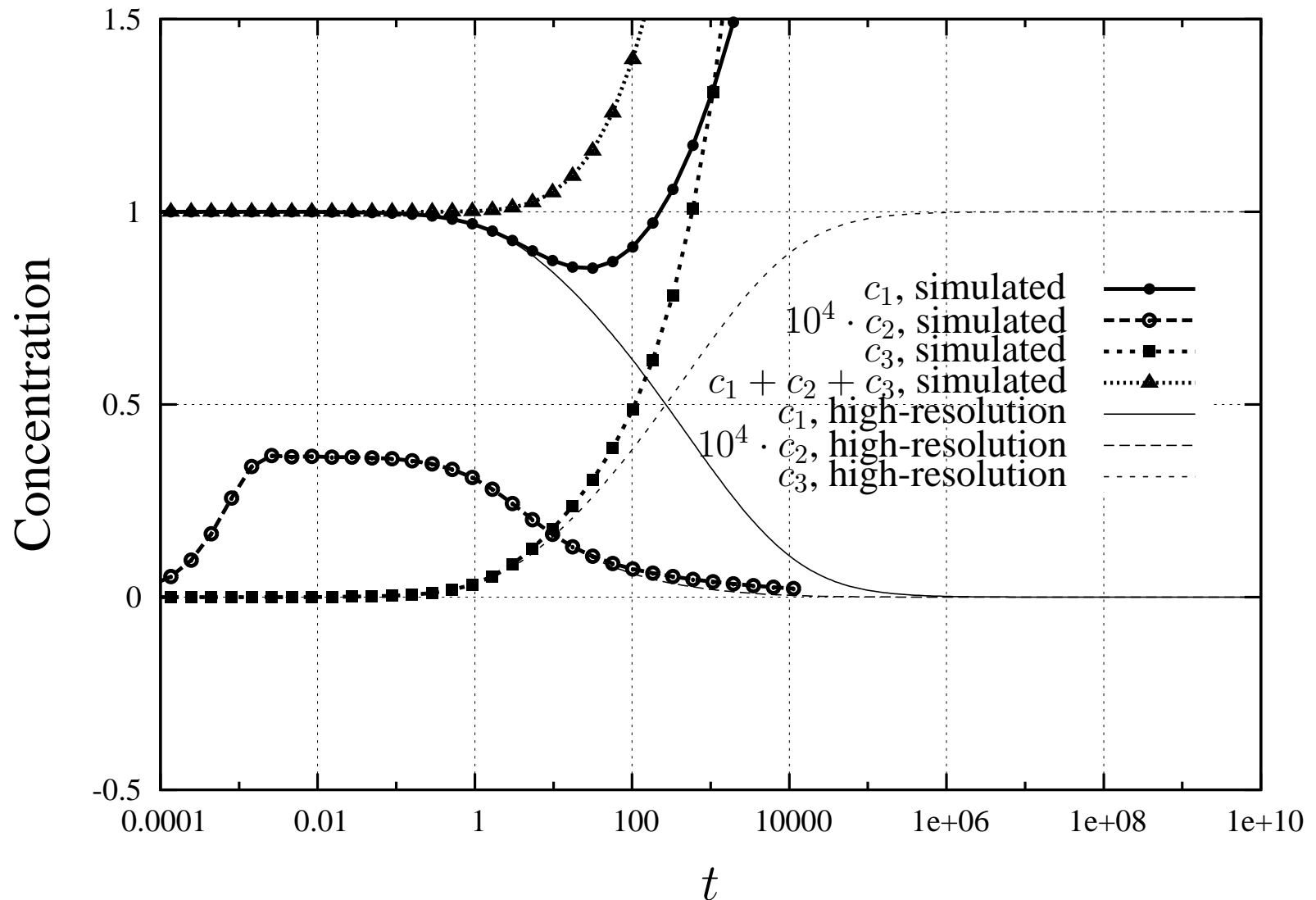
$$c_i^{n+1} = c_i^n + \Delta t \left( \sum_{j=1}^I p_{i,j}(\bar{c}^n) \frac{c_j^{n+1}}{c_j^n} - \sum_{j=1}^I d_{i,j}(\bar{c}^n) \frac{c_i^{n+1}}{c_i^n} \right), \quad i = 1, \dots, I \quad (58)$$

- Das Verfahren ist konservativ (trivial)
- Das Verfahren ist nicht-negativ (siehe *Burchard, Deleersnijder, Meister* [2003])

Nach dem Runge-Kutta-Prinzip können konservative und nicht-negative Verfahren beliebig hoher Ordnung konstruiert werden.

# mod. Patankar-Trick

## Patankar Runge-Kutta scheme



# mod. Patankar-Trick

## Modified Patankar Runge-Kutta scheme

