Numerische Verfahren zur Lösung partieller Differentialgleichungen in der Physikalischen Ozeanographie

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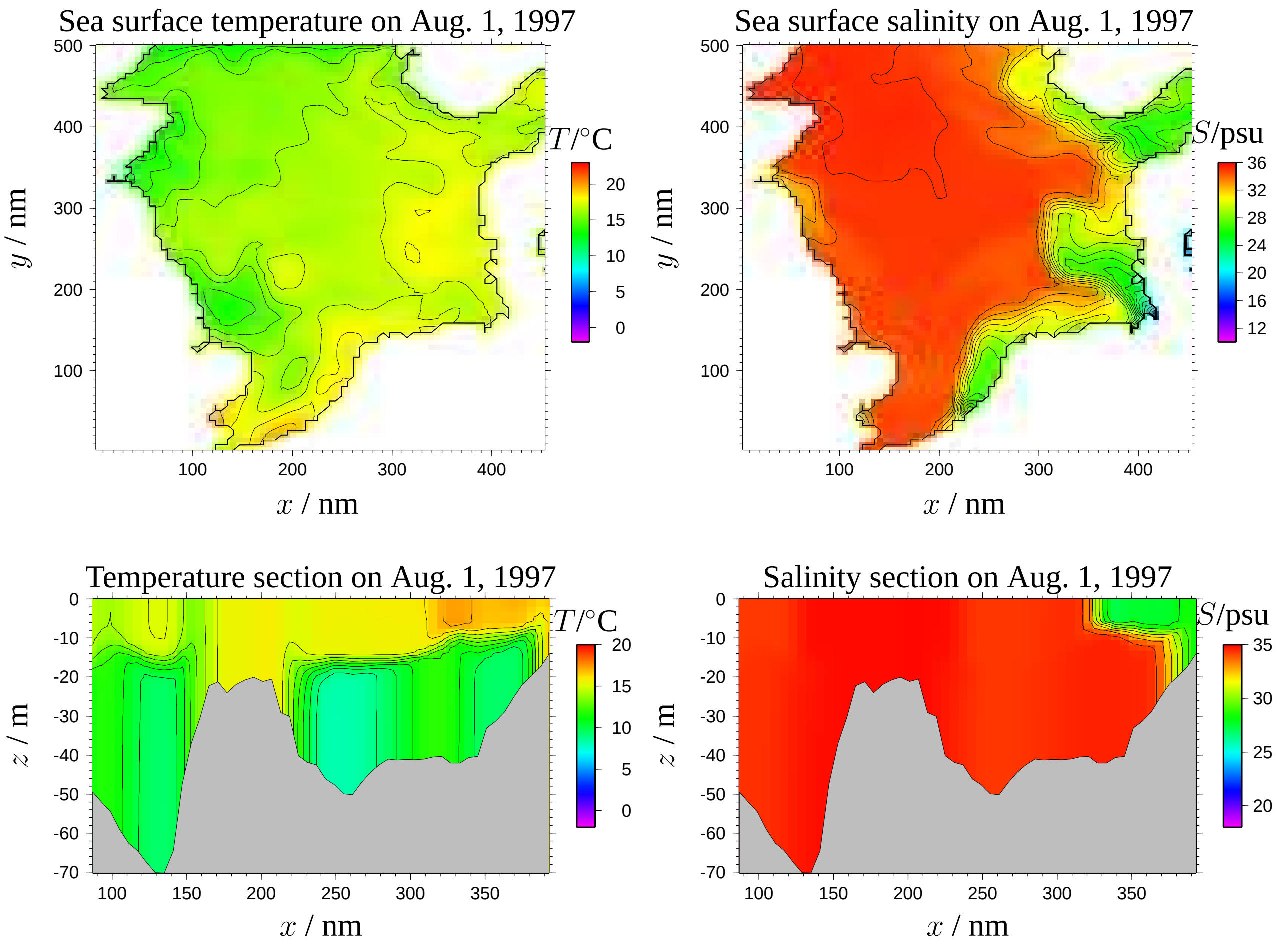
Nordsee-Simulation



SSS in North Sea / Baltic Sea, 1997

u-Gleichung

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

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

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

$$
b = -g\frac{\rho-\rho_0}{\rho_0} \tag{2}
$$

v-Gleichung

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

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

$$+fu \quad \underbrace{-\int_z^\zeta \partial_y b\, dz'}_{\text{Druckgradient (1)}} \quad = -\partial_y\left(g\zeta + \frac{1}{\rho_0}p_0\right). \tag{3}$$

Kontinuitätsgleichung

Kontinuität:

$$\partial_x u + \partial_y v + \partial_z w = 0. \tag{4}$$

Freie Oberfläche:

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

mit

$$U = \int_{-H}^{\zeta} u\, dz, \qquad V = \int_{-H}^{\zeta} v\, dz. \tag{6}$$

Tracer-Gleichung

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

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

$$\rho = \rho(c^1, c^2, \ldots, c^N, p_0) \tag{8}$$

Turbulenz-Modell

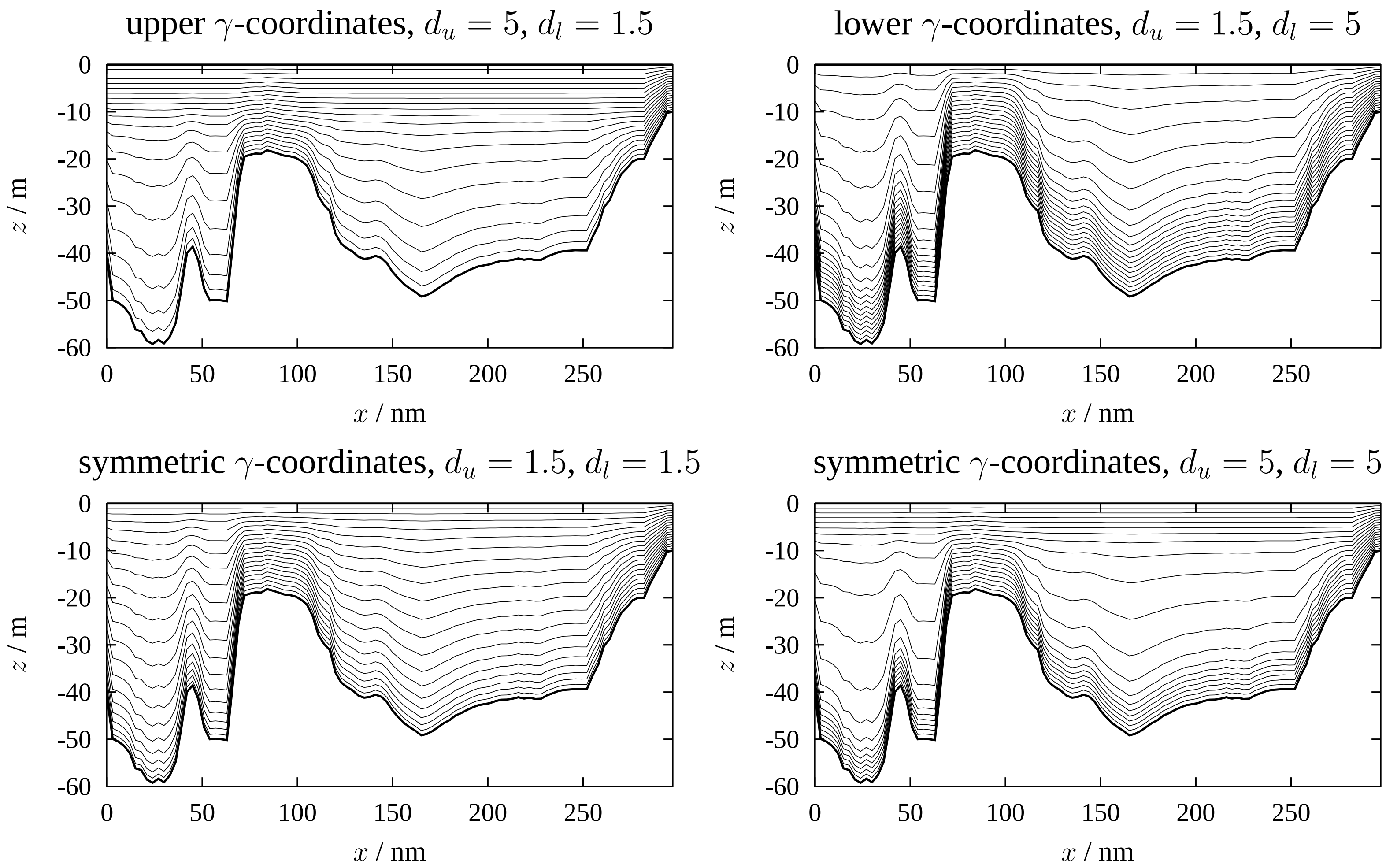
$$\partial_t k - \partial_z \left(\left(\nu + \frac{\nu_t}{\sigma_k} \right) \partial_z k \right) = P + B \underbrace{-\varepsilon}_{\text{Patankar (5)}} , \qquad (9)$$

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

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

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

Vertikale Koordinaten



Schichtgemittelte Gleichungen

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

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

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

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

Dichtegradient, diskret

$$(\partial_x^* b)_k = \frac{1}{2}(\partial_x b_{k+1} + \partial_x b_k) - \partial_x z_k \frac{b_{k+1} - b_k}{\frac{1}{2}(h_{k+1} + h_k)}$$

$$\sim \frac{\frac{1}{2}(b_{i+1,k+1} + b_{i+1,k}) - \frac{1}{2}(b_{i,k+1} + b_{i,k})}{\Delta x} \qquad (15)$$

$$-\partial_x z_k \frac{\frac{1}{2}(b_{i+1,k+1} + b_{i,k+1}) - \frac{1}{2}(b_{i+1,k} + b_{i,k})}{\frac{1}{2}(h^c_{i,k} + h^c_{i+1,k})}$$

Hydrostatische Konsistenz

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

$$-\frac{(\frac{1}{2}+\alpha)b_{i,k+1} + (\frac{1}{2}-\alpha)b_{i,k}}{\Delta x} \tag{16}$$

$$\alpha = \frac{\partial_x z_k \Delta x}{h^c_{i,k} + h^c_{i+1,k}}. \tag{17}$$

Hydrostatische Konsistenzbedingung:

$$|\partial_x z_k| \frac{\Delta x}{\frac{1}{2}(h^c_{i,k} + h^c_{i+1,k})} \leq 1. \tag{18}$$

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:

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

Baroklines Zeitschrittkriterium:

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

Lösungsstrategie

Vertikal-integrierte Gleichung:

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

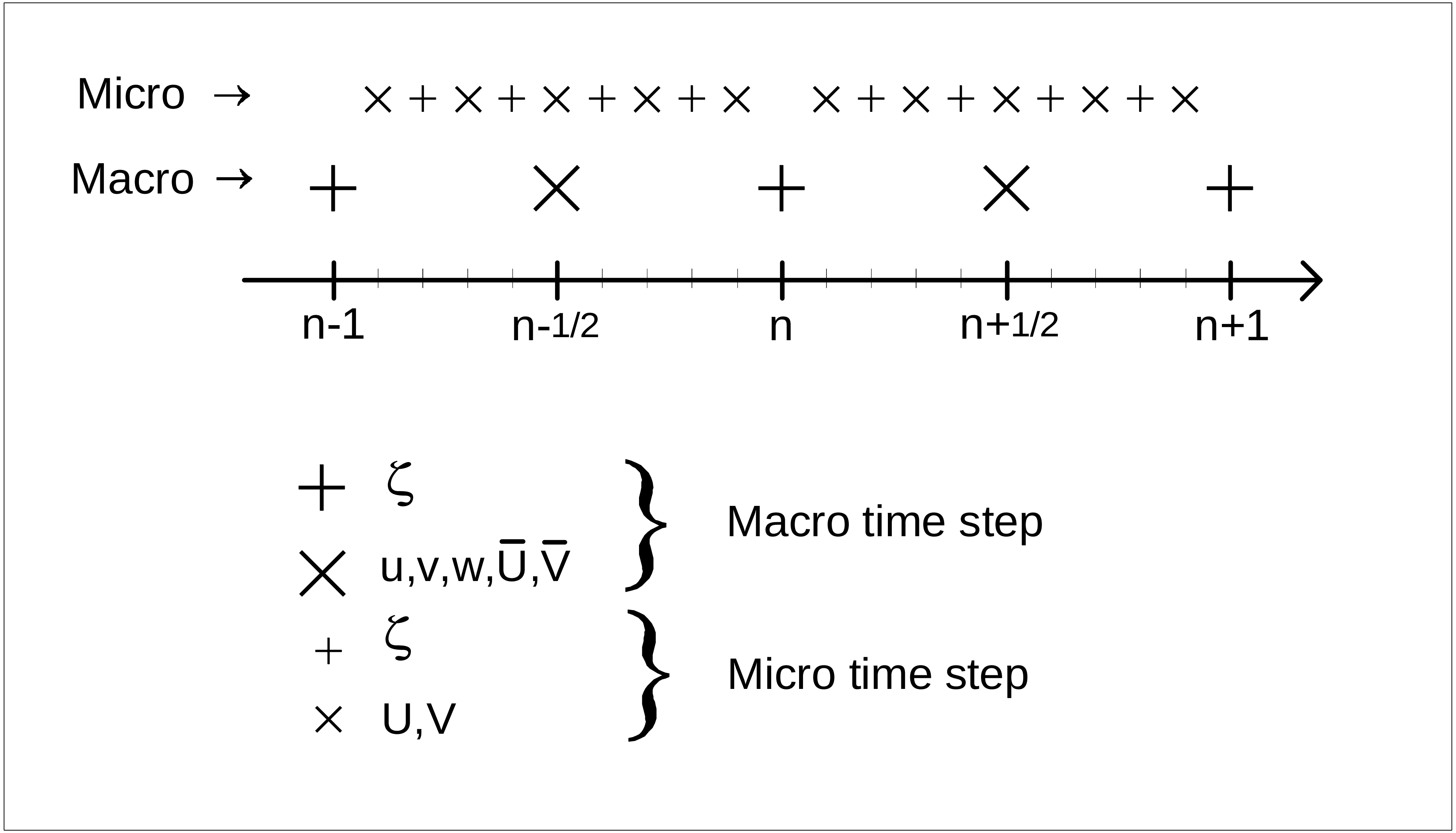
Umformung:

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

Interaktionsterm:

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

Zeitschrittschema



TVD advection schemes I

One-dimensional linear tracer equation:

$$\partial_t \Psi + \partial_x (u\Psi) = 0 \tag{24}$$

Discretisation:

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

Upstream-biased flux calculation:

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

TVD advection schemes II

Polynomial tracer approximation:

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

Lax-Wendroff form:

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

$$\Phi^+_{i+1/2} = \alpha_{i+1/2} + \beta_{i+1/2} r^+_{i+1/2}, \quad \Phi^-_{i+1/2} = \alpha_{i+1/2} + \beta_{i+1/2} r^-_{i+1/2}, \tag{29}$$

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

$$r^+_{i+1/2} = \frac{\Psi_i - \Psi_{i-1}}{\Psi_{i+1} - \Psi_i}, \quad r^+_{i+1/2} = \frac{\Psi_{i+2} - \Psi_{i+1}}{\Psi_{i+1} - \Psi_i}. \tag{31}$$

TVD advection schemes III

P$_2$-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

$$\partial_t(D\Psi) + \partial_x(uD\Psi) + \partial_y(vD\Psi) = 0 \tag{35}$$

$$\partial_t D + \partial_x(uD) + \partial_y(vD) = 0 \tag{36}$$

Directional split (Pietrzak [1998])

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

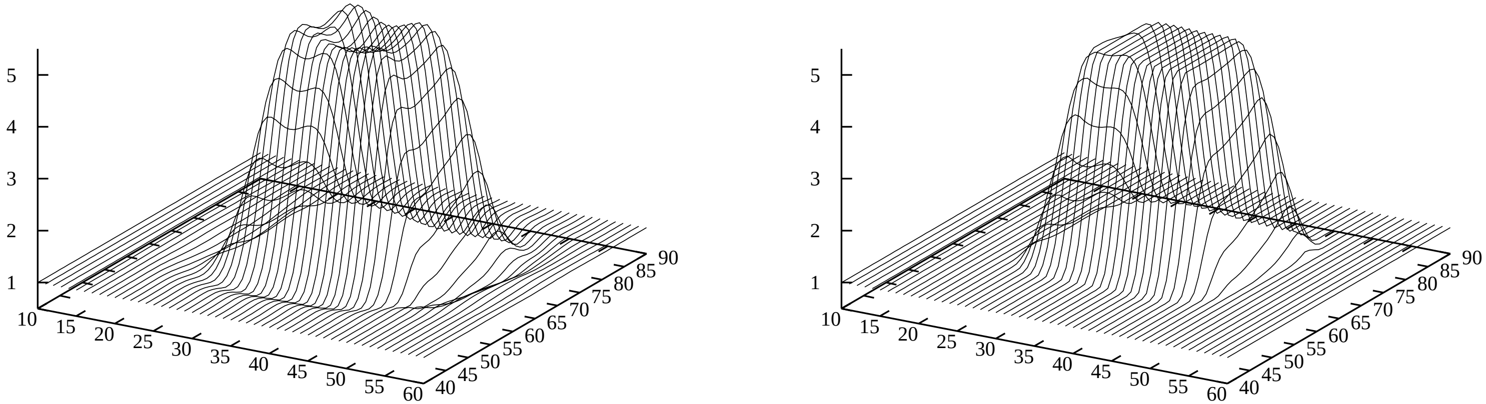
$$D_{i,j}^{n+1}\Psi_{i,j}^{n+1} = D_{i,j}^{n+1/2}\Psi_{i,j}^{n+1/2} - \frac{\Delta t}{\Delta y}(D_{i,j+1/2}^{n}F_{i,j+1/2}^{n} - D_{i,j-1/2}^{n}F_{i,j-1/2}^{n}) \tag{38}$$

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

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

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:

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

Diskret (Crank-Nicolson):

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

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

Energieerhaltung

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

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

Diskret:

$$\frac{\hat{e}_j - e_j}{\Delta t} - \frac{\nu_{j+1/2}\frac{\bar{e}_{j+1}-\bar{e}_j}{z_{j+1}-z_j} - \nu_{j-1/2}\frac{\bar{e}_j-\bar{e}_{j-1}}{z_j-z_{j-1}}}{z_{j+1/2}-z_{j-1/2}} =$$

$$-\frac{1}{2}\nu_{j+1/2}\frac{\sigma(\hat{u}_{j+1}-\hat{u}_j)(\hat{u}_{j+1}-u_j)+(1-\sigma)(u_{j+1}-u_j)(u_{j+1}-\hat{u}_j)}{(z_{j+1/2}-z_{j-1/2})(z_{j+1}-z_j)}$$

$$-\frac{1}{2}\nu_{j-1/2}\frac{\sigma(\hat{u}_j-\hat{u}_{j-1})(\hat{u}_j-u_{j-1})+(1-\sigma)(u_j-u_{j-1})(\hat{u}_j-u_{j-1})}{(z_{j+1/2}-z_{j-1/2})(z_j-z_{j-1})}$$

$$=: -P^l_{j+1/2} - P^u_{j-1/2}. \tag{45}$$

Energieerhaltung

Turbulenzproduktion, neu:

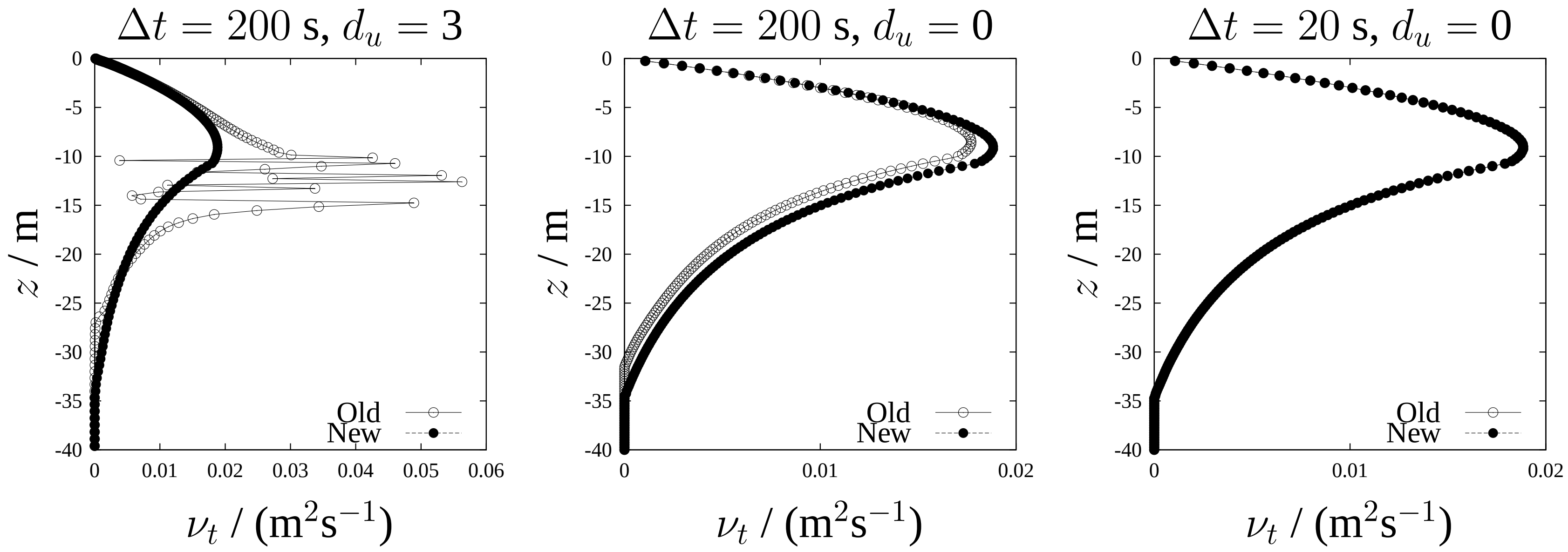
$$P_{j+1/2} \;=\; \nu_{j+1/2}\frac{(\bar{u}_{j+1}-\bar{u}_j)(\tilde{u}_{j+1}-\tilde{u}_j)}{(z_{j+1}-z_j)^2}, \qquad (46)$$

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

Turbulenzproduktion, alt:

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

Energieerhaltung



Patankar-Trick

$$\partial_t X = P - QX, \quad P, Q > 0 \tag{48}$$

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

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

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

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

mod. Patankar-Trick

Test-Problem:

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

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

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

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

mod. Patankar-Trick

$$\sum_{i=1}^{I}(P_i(\vec{c}) - D_i(\vec{c})) = \qquad (57)$$

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

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:

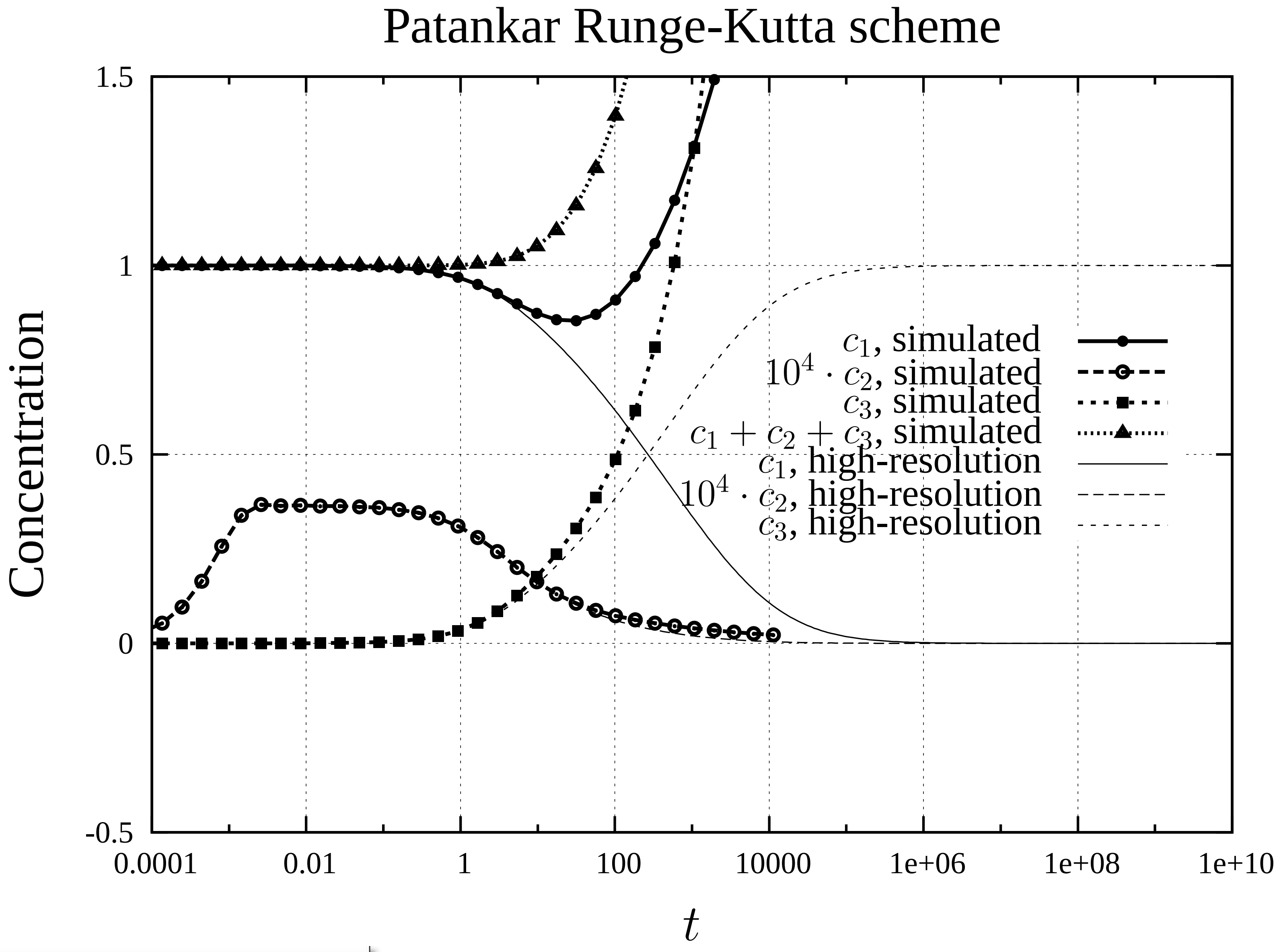
modifiziertes Patankar-Euler-Verfahren:

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

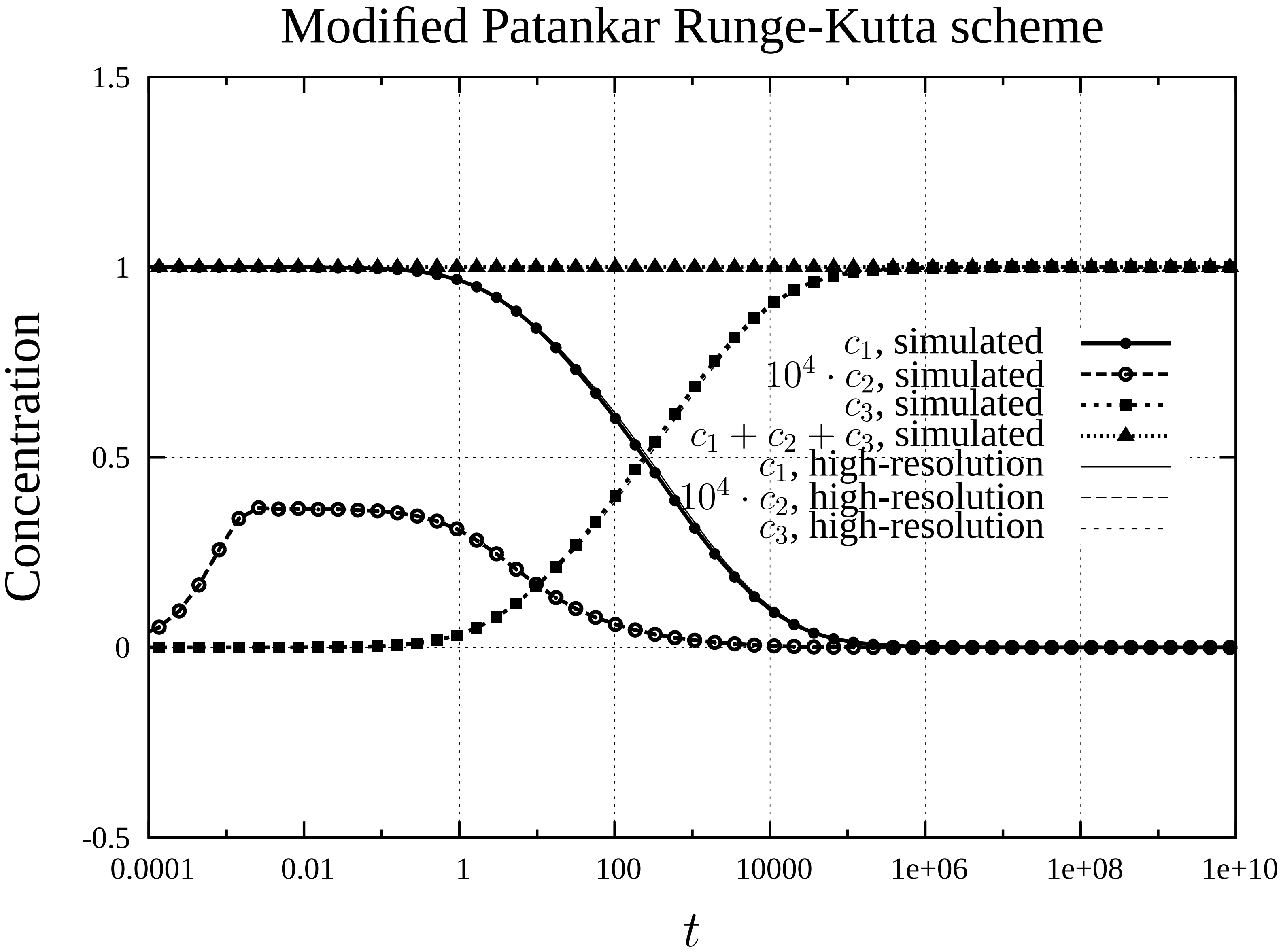
- Das Verfahren ist konservativ (trivial)
- Das Verfahren ist nicht-negativ (siehe *Burchard, Deleersnijder, Meister* [2003])

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

mod. Patankar-Trick



mod. Patankar-Trick



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