Numerical aspects in offline coupling of biochemical reaction modules with advection-diffusion simulations

1. Introduction

2. how we couple computations offline

3. how we control the numerical approximation

4. Summary

BfG - Federal Institute of Hydrology
scientific decision support for german waterways administration

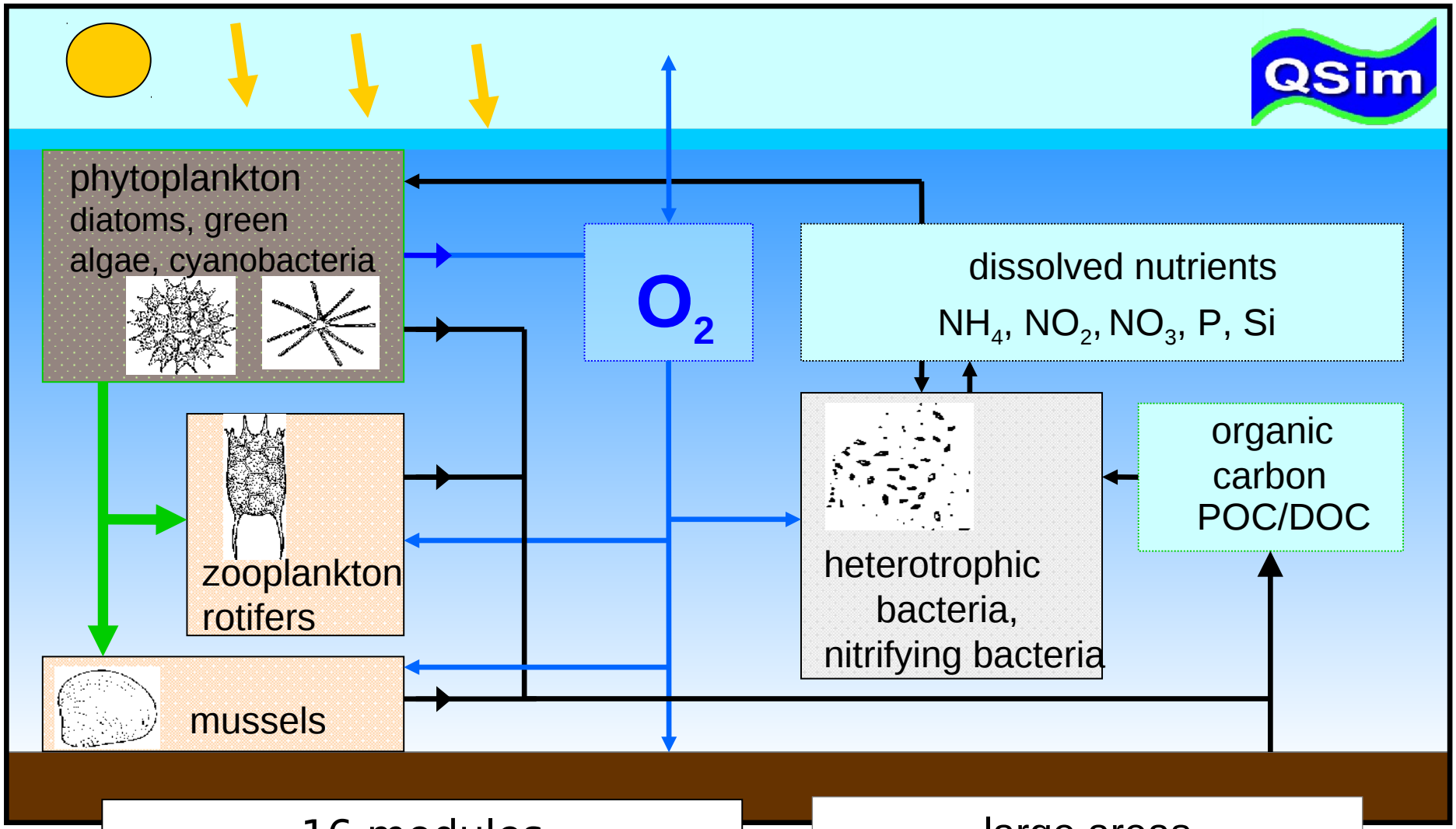
our team: water quality modelling

25 years of experience in: 1D cross-section averaged modelling
offline-coupling via flow-field

currently under development: 2D/3D modelling for estuaries
T-QSim

concern: water quality problems in german north sea estuaries

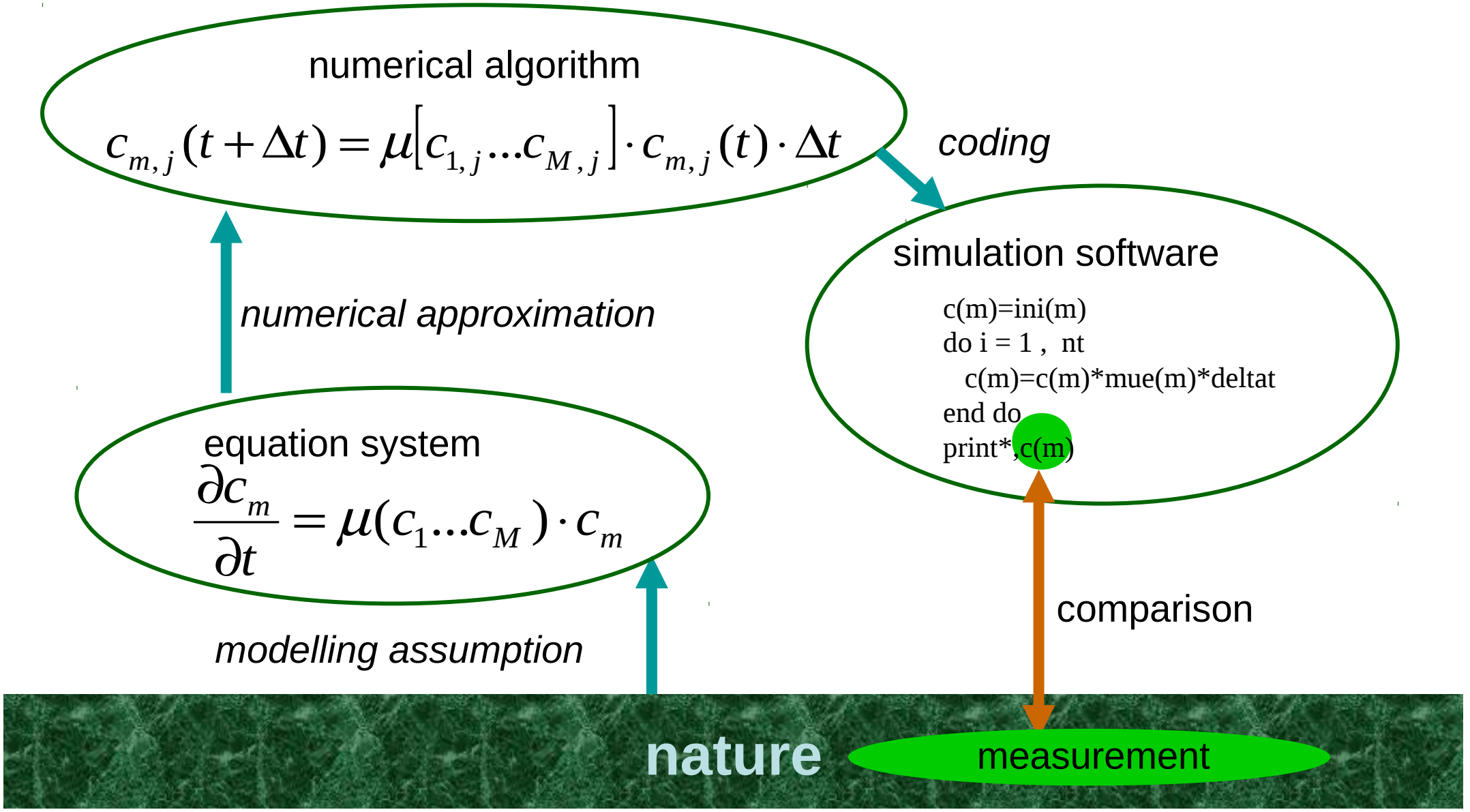
Oxygen budget



16 modules
70 planctic concentrations
100 empiric parameters

large areas
long time-intervals
lots of calibration runs

3 modelling steps



transport equation

fluid dynamics (RANS)

biochemical reactions

$$\frac{\partial c_m}{\partial t} = \underbrace{- v_i \frac{\partial c_m}{\partial x_i}}_{advection} + \underbrace{\frac{\partial}{\partial x_i} D_{ij} \frac{\partial c_m}{\partial x_j}}_{diffusion} + \underbrace{Q_m(c_1 \ldots c_m \ldots c_M, x_i, t)}_{source} - \underbrace{w_{s,3} \frac{\partial c_m}{\partial x_3}}_{settling/rise}$$

time-integration

$$c_m(t + \Delta t, \underline{x}) = c_m(t, \underline{x}_{orig}) + \Delta c_m^{diff} + \Delta c_m^{react}$$

concentration next timestep at location x

concentration previous timestep at origin of streamline

change due to diffusion

change due to reaction / metabolism

coupling numerics and software

computational fluid dynamics, hydraulic model, software SELFE
casu ...

streamline backtracking
ELM

turbulence
model

$$c_m(t+\Delta t, \underline{x}) = c_m(t, \underline{x}_{orig}) + \Delta c_m^{diff} + \Delta c_m^{react}$$

offline storage

fractional step algorithm

$$c_{m,k}(t+\Delta t) = A_{kl}(\Delta t^{adv}) c_{m,l}^{diff,react} \quad ; \quad c_{m,k}^{diff,react} = D_{kl}(\Delta t^{diff}) c_{m,l}^{react} \quad ; \quad c_{m,k}^{react} = Q_m(c_1(t) \dots c_M(t), \underline{x}, t, \Delta t^{react})$$

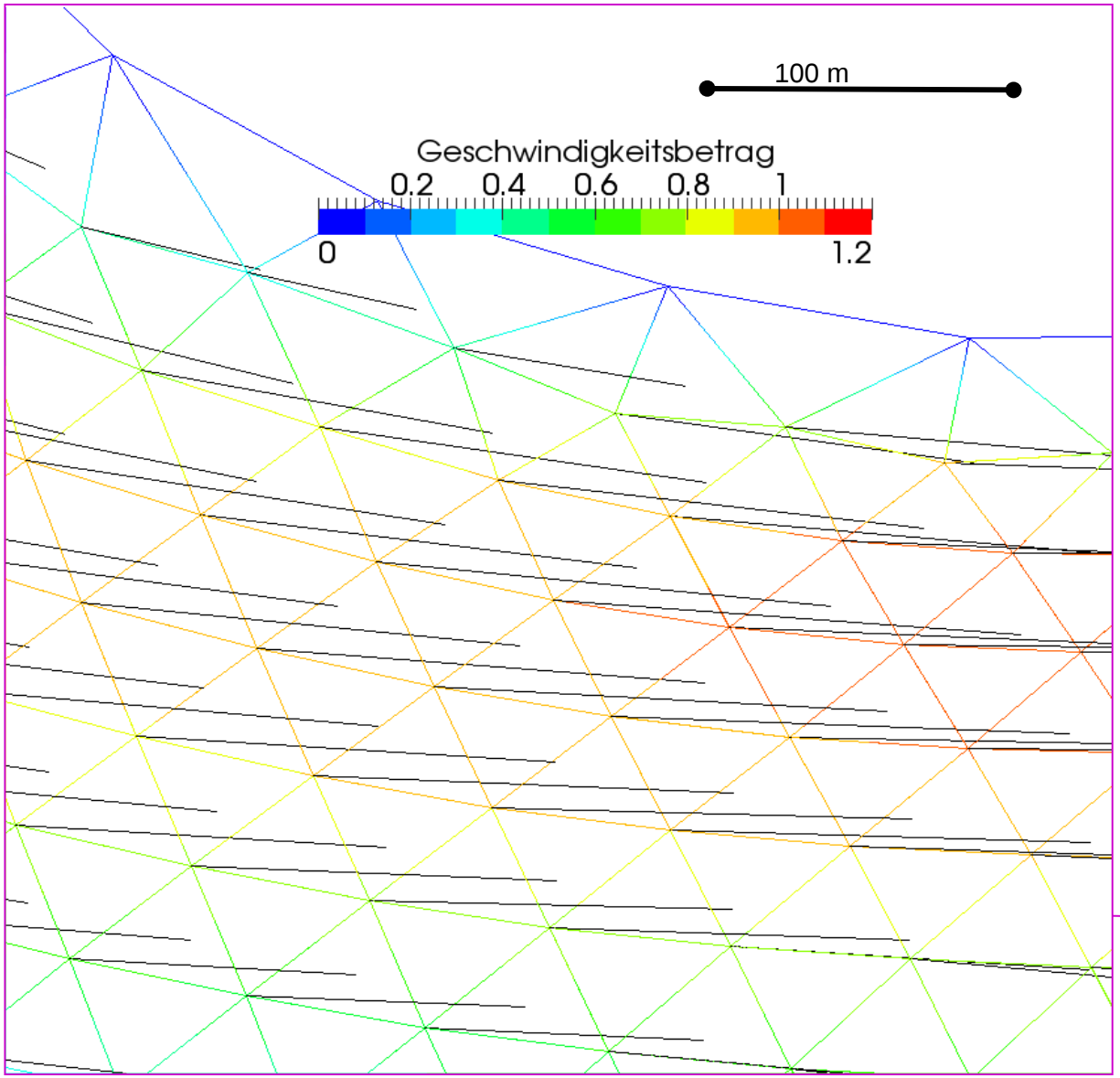
$$n_1 \cdot \Delta t^{adv} = n_2 \cdot \Delta t^{diff} = \Delta t^{react}$$

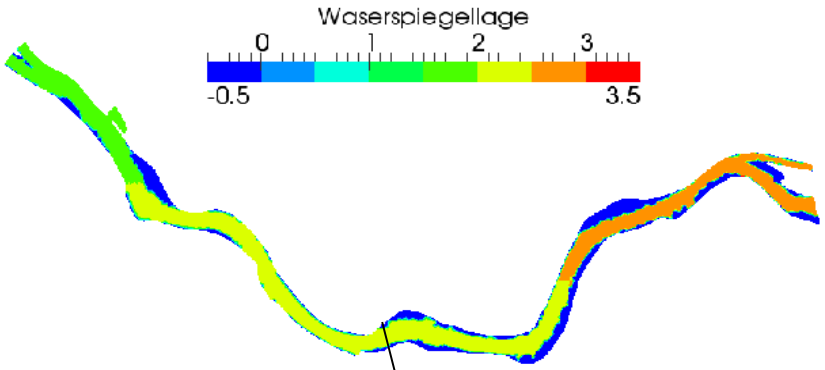
Water quality simulation, software T-QSim

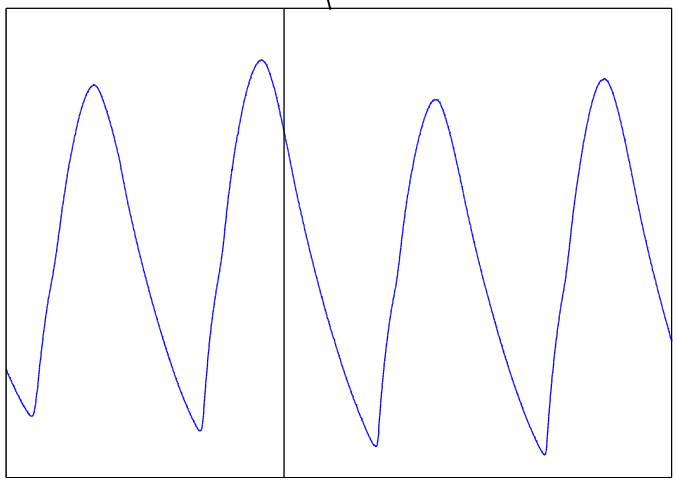
Zeitpunkt 318412950s (2010-feb-01 08:02:30 Uhr)

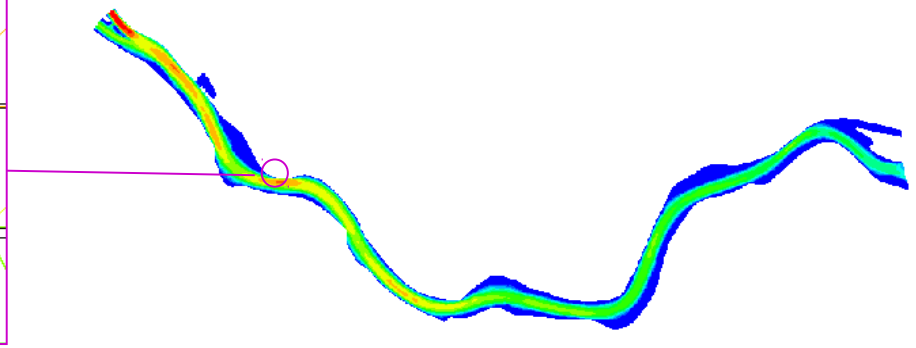
Teilmodell Elbe Ästuar Bunthaus-Geesthacht

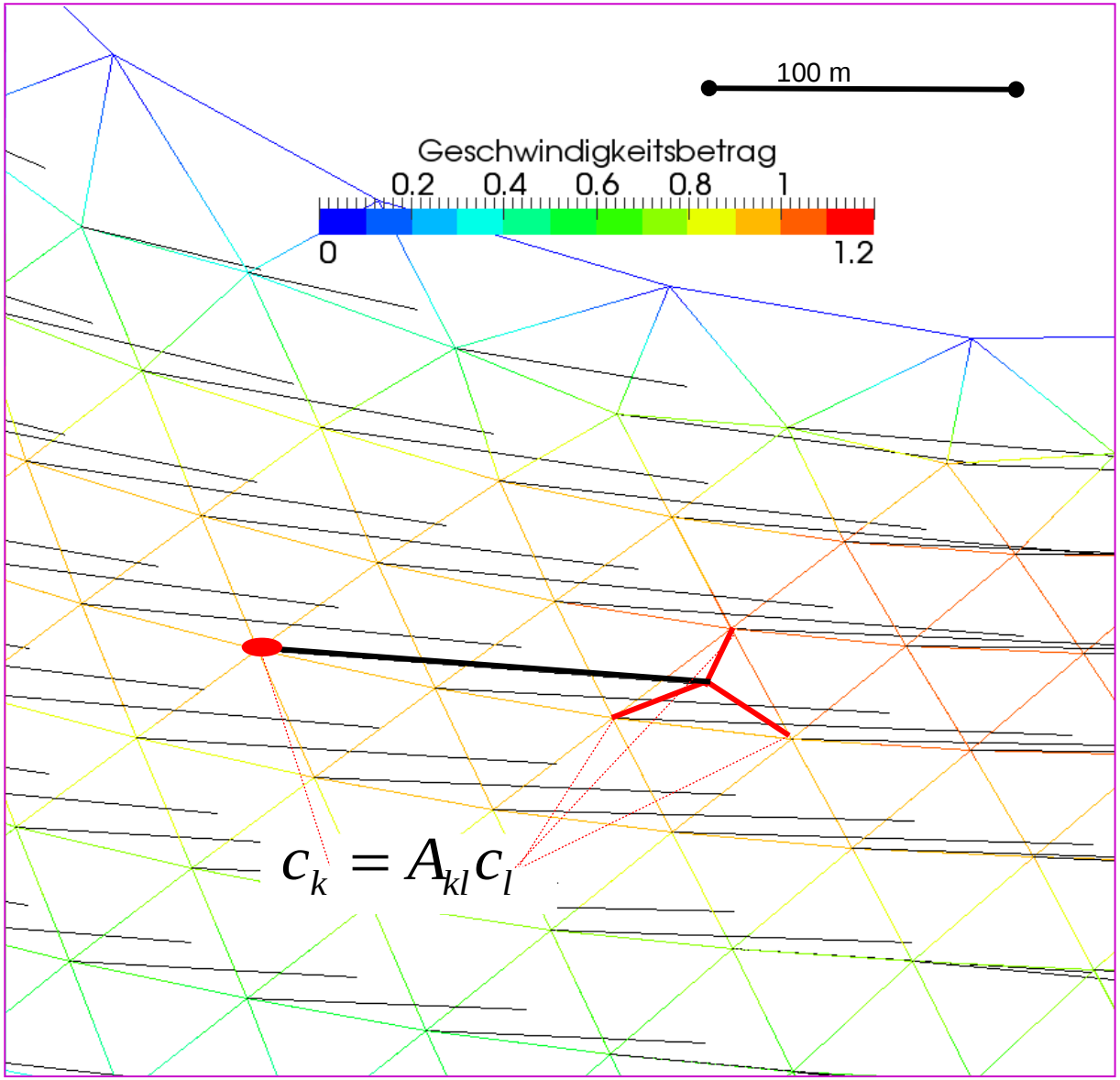
casu Rechenlauf gebu2 02sep13 dt=150s







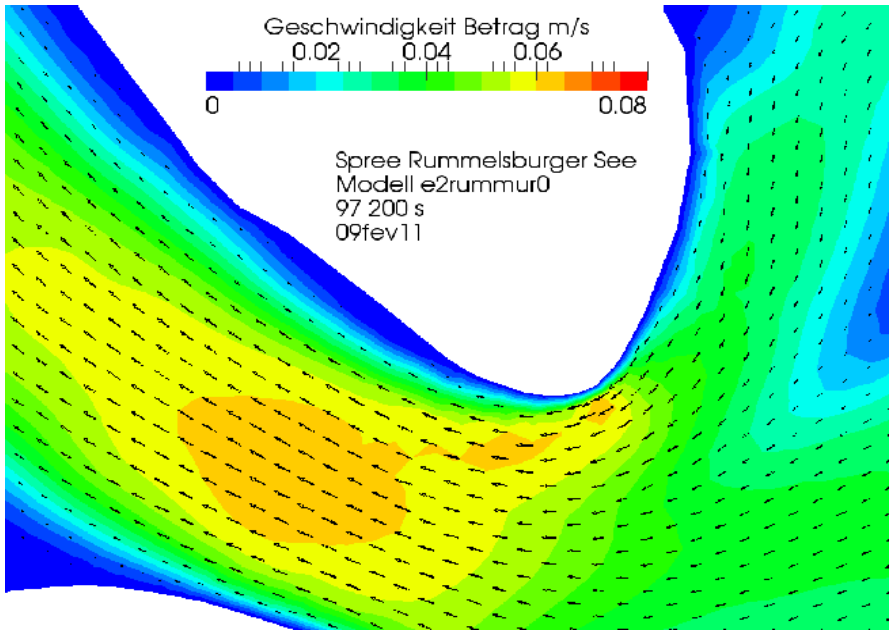


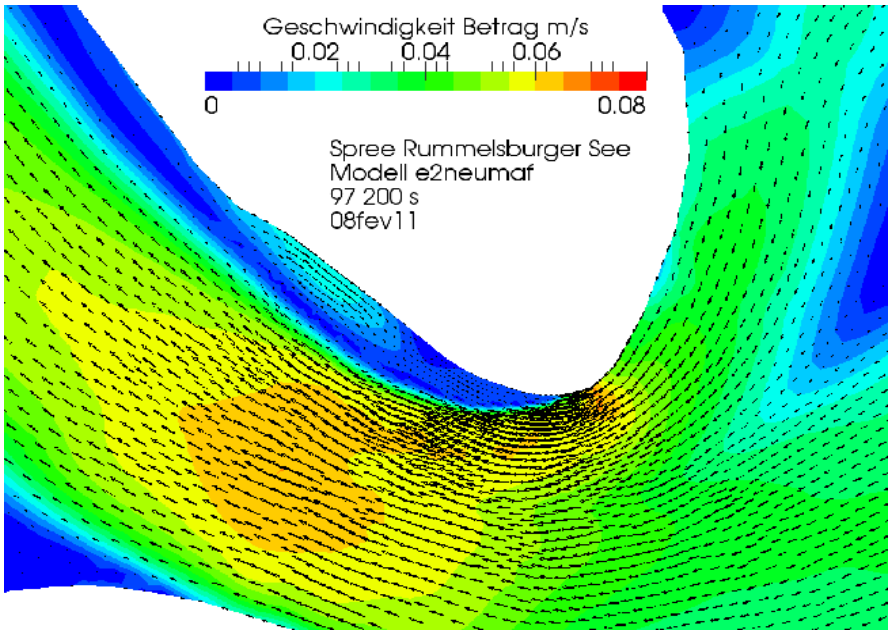


Advection Matrix A contains the weighting-factors from interpolation around streamline origin

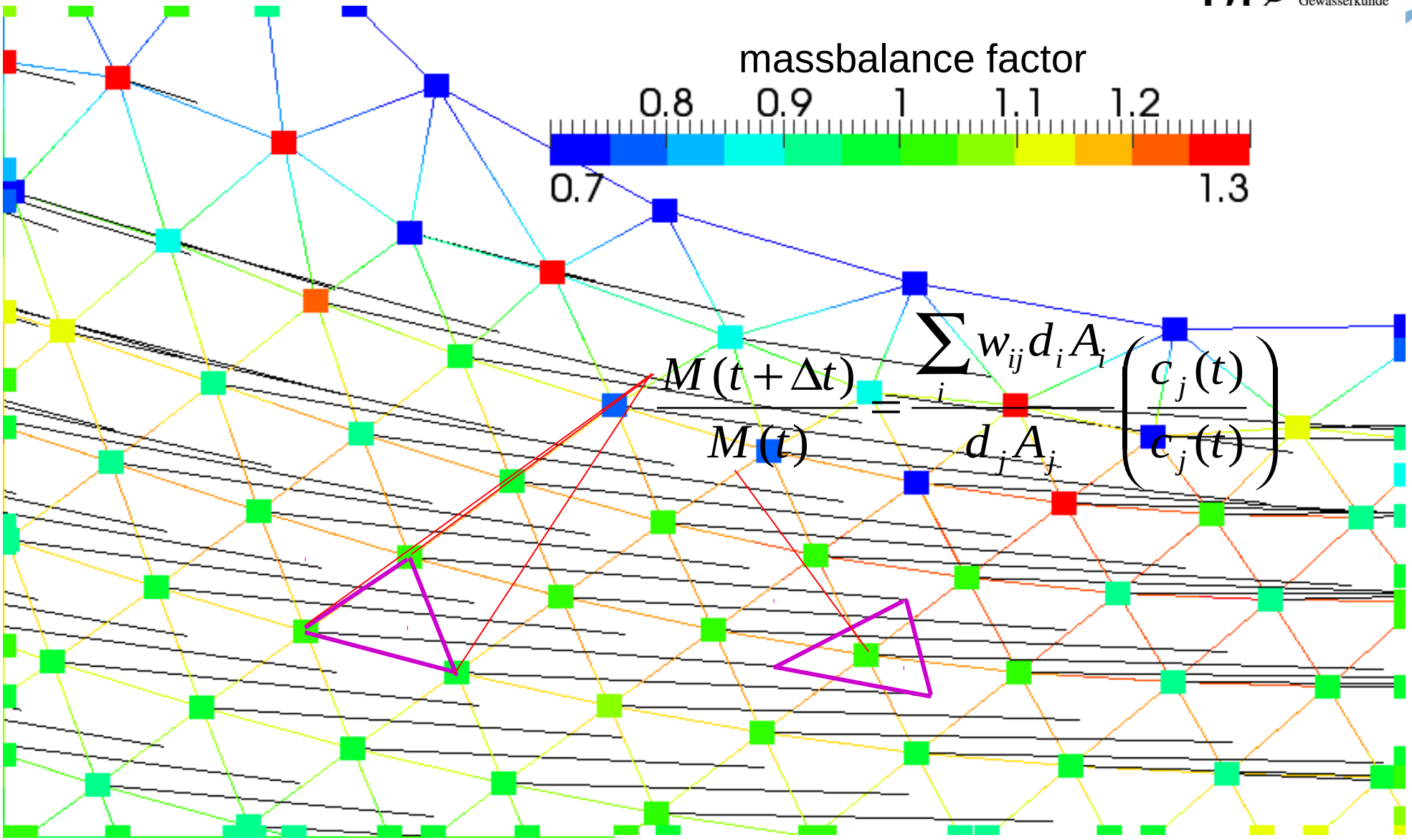
Advection Matrix A is independant of concentration field

control of numerical approximation by grid refinement test





detail of river Spree model,
purpose: pedicting the area influenced by a heat discharge
refinement allows for prediction of recirculation zone
but: does not change the conclusion

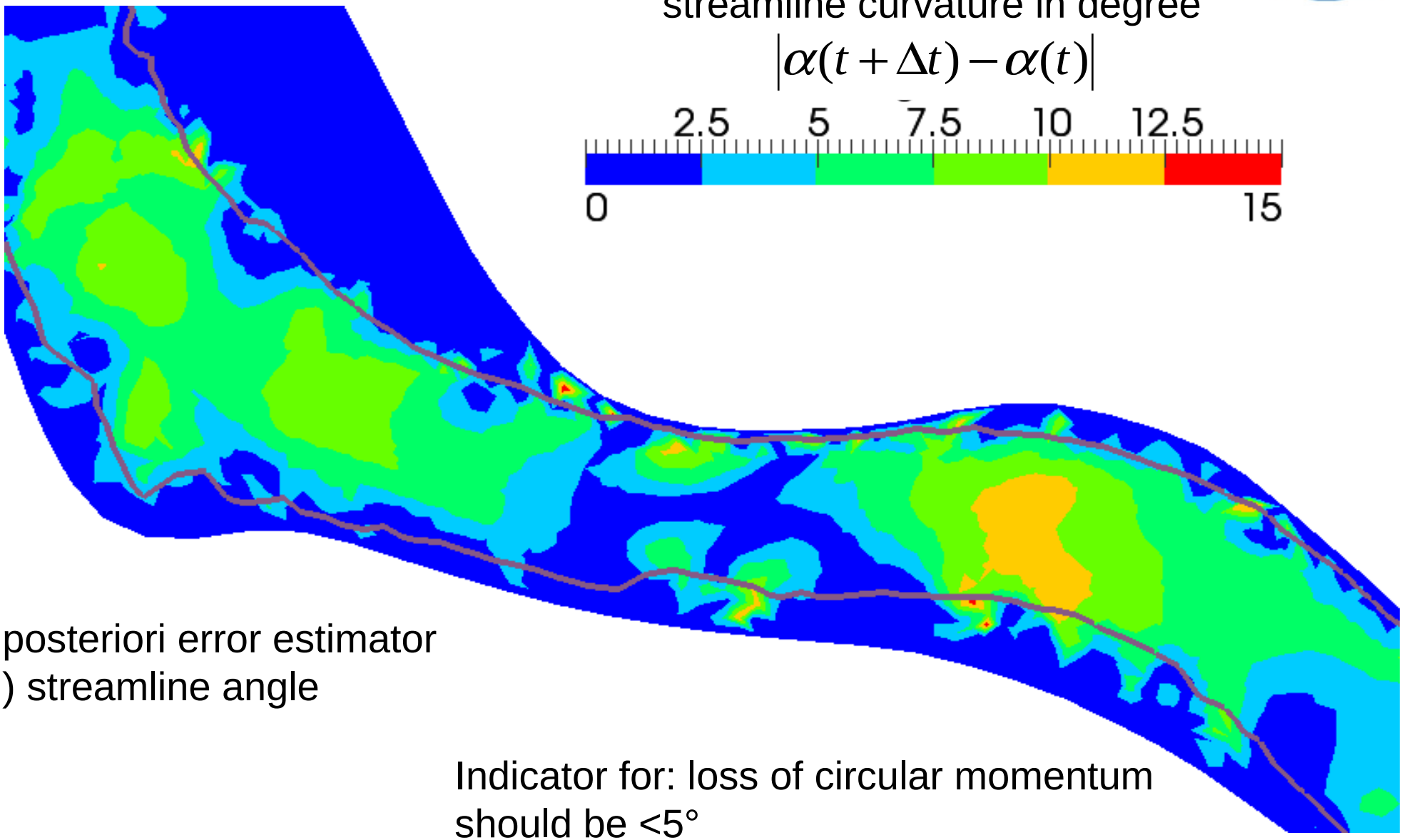


a posteriori error estimator
1.) massbalance factor

Indicating: local errors in mass balance
needs to be combined with integral measures
remedy: correction algorithm

streamline curvature in degree

$$\left|\alpha(t+\Delta t)-\alpha(t)\right|$$

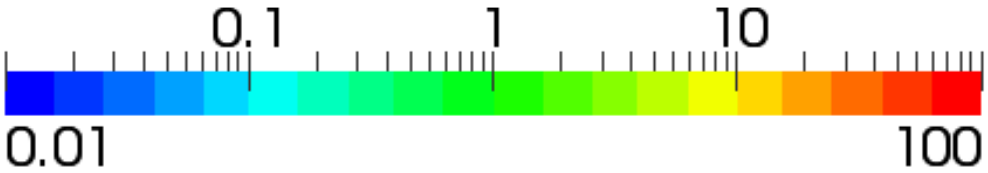


a posteriori error estimator
2.) streamline angle

Indicator for: loss of circular momentum
should be <5°
remedy: shorter timestep

max. scaled numerical diffusivity

$$\frac{\nu_{num.}}{\nu_{Elder}} \leq \frac{\Delta x^2 / \Delta t}{= 5.93 \cdot v_\tau \cdot d}$$



a posteriori error estimator
3.) numerical diffusivity

Indicator for: unrealistic mixing
remedy: finer mesh, larger time-step

take home message

1. Coupled algorithms do need more attention and creativity to check the accuracy of numerical approximation.

2. There is a higher benefit in **controll** of numerical accuracy than in **improvement** of numerical accuracy.

3. We do see a need to develop methods to control numerical accuracy of coupled models