Software Coupling shaped by Organisational Needs in Interdisciplinary Research

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BfG Federal Institute of Hydrology

Overview

Introduction:
- personal career in RSE
- institutonal history of RSE

Organisational Needs in Interdisciplinary Research

Choices on software design:
- offline coupling
- rewrite <-> refactoring
- open-source developer communities

Resume

my personal career as a RSE

1984-1991	TU Berlin, pysikalische Ingenieurwissenschaften, 4 student projects on numerical simulation including software development, team work and project management
1992-1997	river enineering consultant company applying and developing flood flow simulations
1997-2003	Ph.D. on turbulence simulation for density stratified flows applied to fluid mud (dense suspended sediment) in estuaries own 3D-code + test strategy
2003-2011	self-employed in computational simulation of river flows
2011-now	RSE supporting the team for microbial ecology at federal institut of hydrology

RSE position paper (Foundational Competencies and Responsibilities of a Research Software Engineer, Goth et al. 2024) is o.k. (software, research, communication)

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Education

interdisciplinary

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Numerics

our institutonal history of RSE

BfG giving scientific advice to german federal water and shipping administration

water quality modelling mainly for german waterways

usage: 3-5 projects in our department, 2 departments inhouse, 4 external users

1979-2018	Volker Kirchesch	starting QSim1D
2011-2030	Jens Wyrwa	starting QSim3D
2022-????	Michael Schönung	rewrite QSim1D

Katerbow, Matthias; Feulner, Georg (2018): Handreichung zum Umgang mit Forschungssoftware. http://doi.org/10.5281/zenodo.1172970 is a great help

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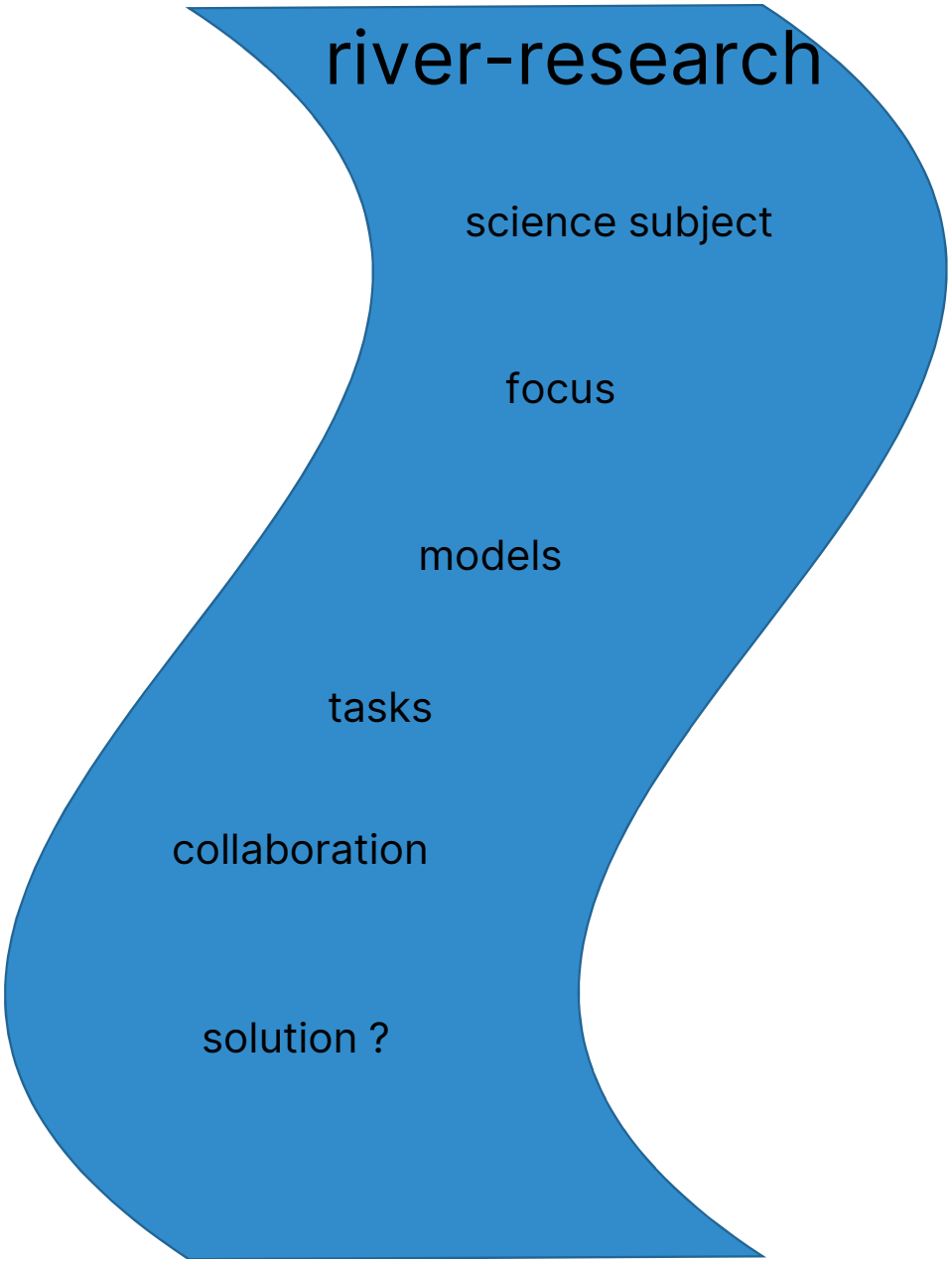

physics + engineering:

fluid dynamics
soil mechanics

shipping
flood hazards

computational fluid dynamics

plan waterways ecologically responsible

need ecological impact

use well established water quality software from trustworthy colleagues

bio-geo-chemistry:

biology
chemistry

environment conservation
nature conservation
human health

model metabolism (Carbon, oxygen, nutrients)

find hypoxia, harmful algael blooms

need flow + transport

use well established hydraulic software from trustworthy colleagues


groins in Elbe river between Lauenburg and Boitzenburg
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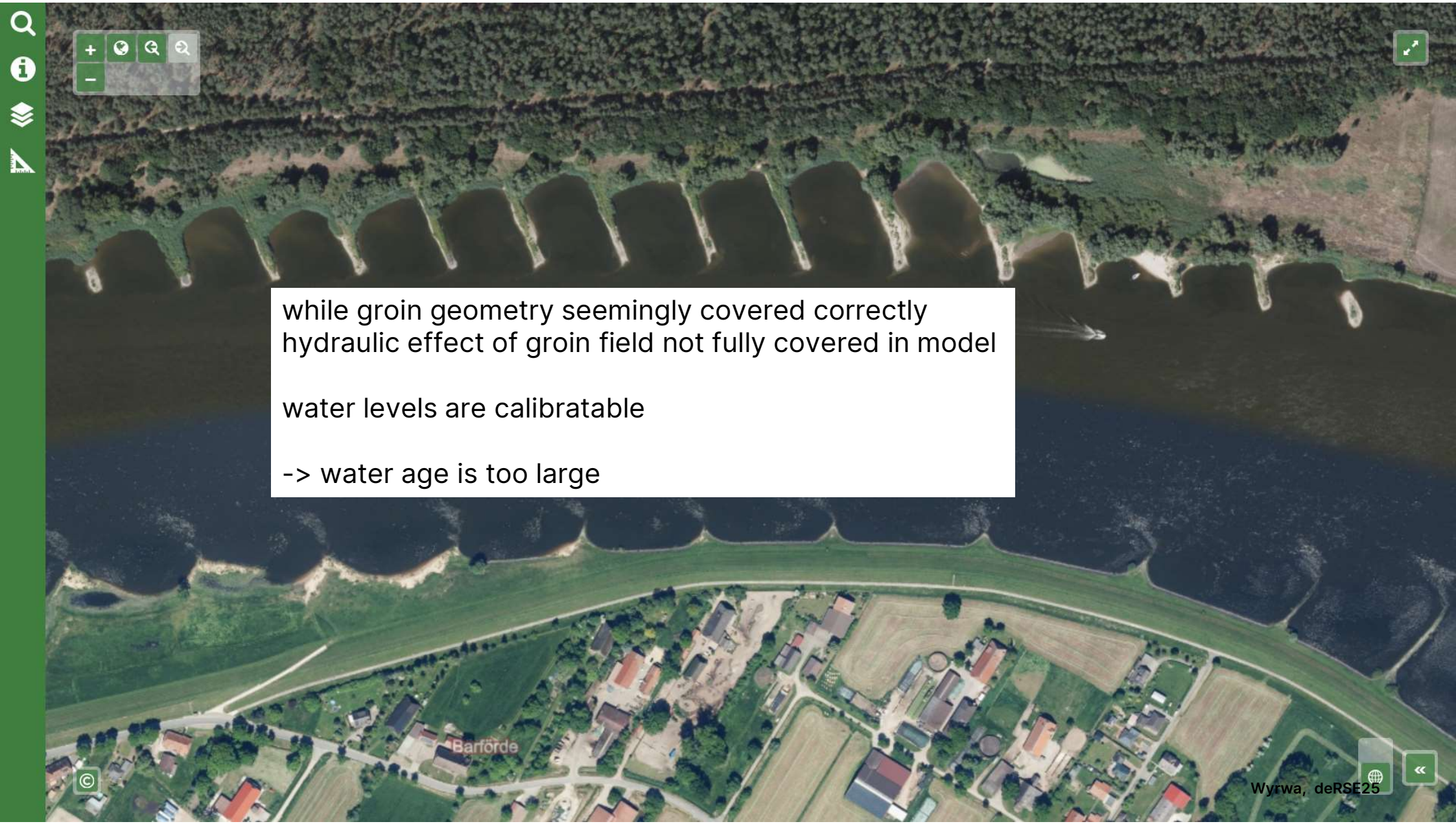
while groin geometry seemingly covered correctly
hydraulic effect of groin field not fully covered in model
water levels are calibratable
-> water age is too large
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gaining speed by offline couping

1 flow simulation + 1 water quality simulation :

offline 201 s

online 180 s

1 water quality simulation if flow field is present :

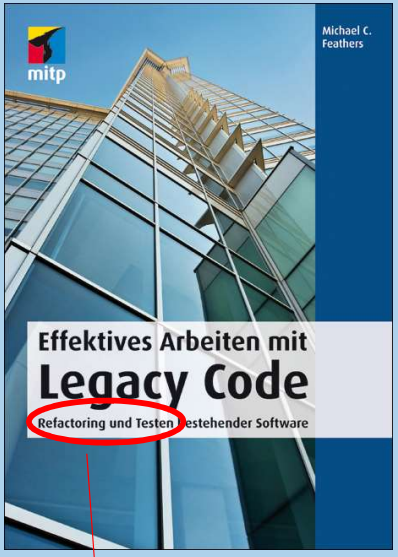
offline 64 s

typical workload in an investigation:

2 flow simulation + 20 water quality simulation

offline 1554 s

online 3600 s



Arbeiten mit Legacy Code ist ein häufiges und bekanntes Phänomen in der Software-Entwicklung.

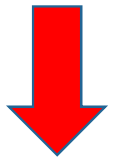
Effektives Arbeiten mit Legacy Code
Refactoring und Testen bestehender Software
Feathers, Michael
Heidelberg : mitp, 2011

Arbeitsrichung:

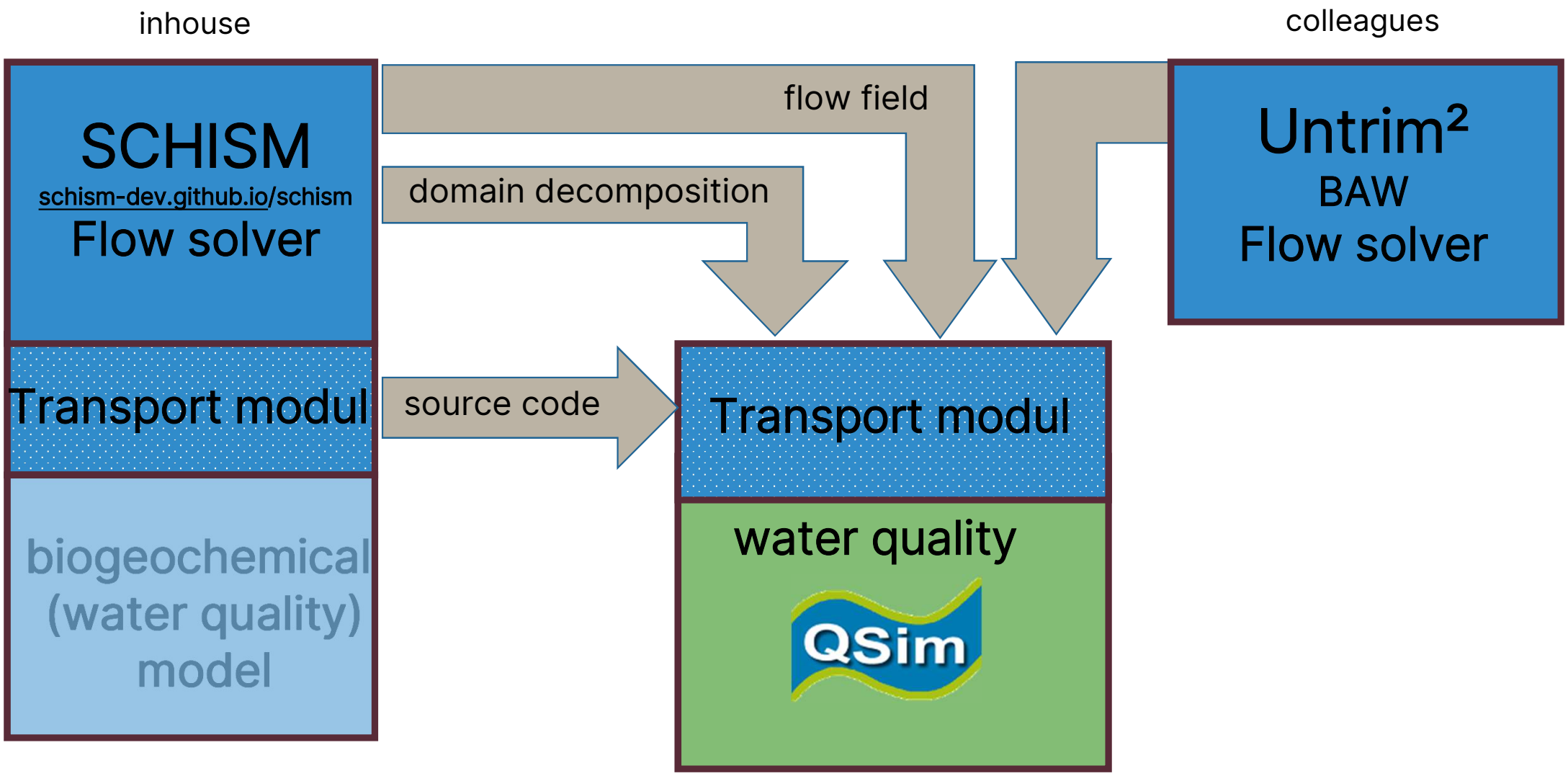
- Refactoring (*funktionsgleiche Entflechtung/Strukturverbesserung)*
- Testen "Es ist wichtig, den Code unter Testkontrolle zu bringen, bevor Sie ihn modifizieren"

Refactoring im laufenden Betrieb:
Strukturverbesserung, Dokumentation und Testbarkeit gleich herbeiführen, wenn sich der Programmteil in der Bearbeitung befindet.

refactoring modules



full rewrite of core


inhouse
colleagues
SCHISM
schism-dev.github.io/schism
Flow solver
Transport modul
biogeochemical (water quality) model
flow field
domain decomposition
source code
Untrim²
BAW
Flow solver
Transport modul
water quality
QSim

all 4 modes of cooperation

do hydraulics ourself and <-> use results from partners (consult with specialists)

work simultaneously <-> work one after another

availability + trust

Summary

offline coupling turned out to be crucial for the success
computing speed + development resources + interdisciplinary collaboration

poor documentation + unsystematic data structures
serious obstacle to further development of legacy code.

The integration into larger open-source software communities
was started and yields promising results.

Different teams or different modes of collaboration
require different coupling options.

Discussion: interdisciplinary teams <-> collaborating teams of specialists

Thank you for your attention.

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