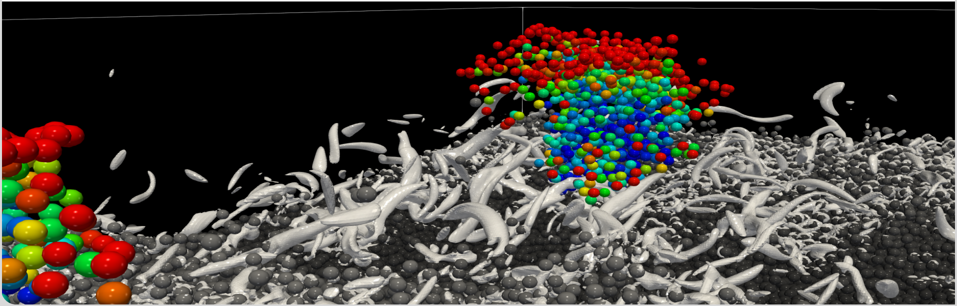
Microorganisms and turbulence

high-performance computing in water quality prediction

7. HPC-Status-Konferenz der Gauß-Allianz

M. Stumpf, M. Uhlmann, M. Pinelli, H. Herlina, J. Qian, H. Horn | 4 Dec 2017

INSTITUTE FOR HYDROMECHANICS (IFH), ENGLER-BUNTE-INSTITUTE (EBI)



Motivation: combined sewer overflow

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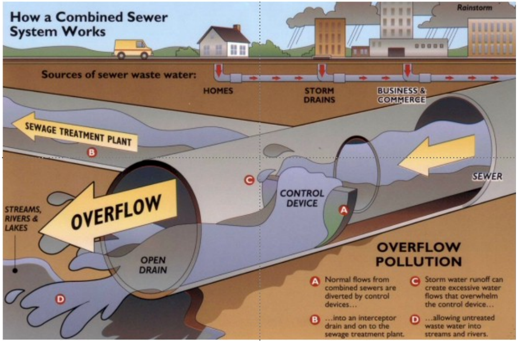
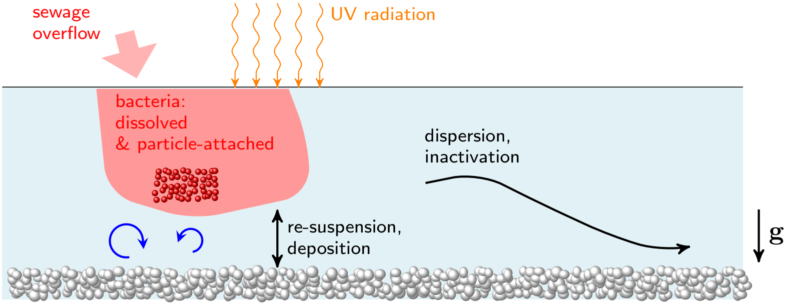
www.dec.ny.gov



wtop.com

www.riverkeeper.org

Model of combined sewer overflow event



- turbulent, open-channel flow with sediment bed
- contamination occurs in dissolved (continuum) and particle-attached (discrete) form
- bacteria population varies due to time, UV radiance, temperature, O_2 concentration, substrate concentration, . . .

Aim of the MOAT project

	current practice	MOAT	challenge
turbulence	RANS	DNS	wide range of scales
particles	continuum	fully resolved	sharp phase interfaces
scalar	neglected	fully resolved	steep gradients
bacteria	modeled	modeled	adaptation of models to higher resolution

- engineering-type models completely neglect inhomogeneities within the problem
- capturing these heterogeneities is computationally very expensive
- MOAT aims to provide a *numerical laboratory* to investigate relevant implications in order to improve engineering-type models

Overview of the methodology

fluid flow

$$\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} + \frac{1}{\rho_f}\nabla p = \nu\nabla^2\mathbf{u} + \mathbf{f_b}$$
$$\nabla\cdot\mathbf{u} = 0$$

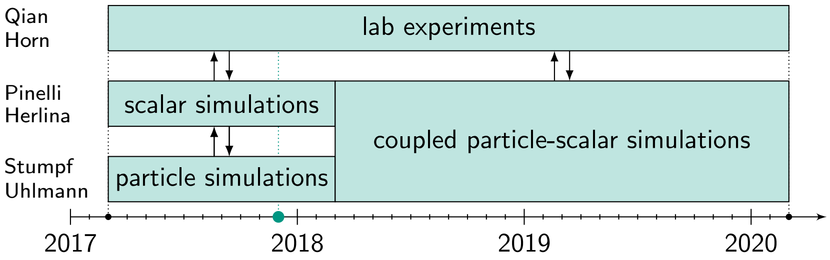
scalar transport

$$\partial_t C_B + (\mathbf{u}\cdot\nabla)\,C_B = D_B\nabla^2 C_B + R_B\,C_B$$
$$\partial_t C_{oxy} + (\mathbf{u}\cdot\nabla)\,C_{oxy} = D_{oxy}\nabla^2 C_{oxy} + R_{oxy}\,C_{oxy}$$
$$\partial_t C_{sub} + (\mathbf{u}\cdot\nabla)\,C_{sub} = D_{sub}\nabla^2 C_{sub} + R_{sub}\,C_{sub}$$
$$\partial_t T + (\mathbf{u}\cdot\nabla)\,T = \kappa\nabla^2 T + q$$

particle motion

$$\rho_p^{(i)} V_p^{(i)}\,\dot{\mathbf{u}}_p^{(i)} = \rho_f \oint_{\partial\mathcal{S}^{(i)}} \boldsymbol{\tau}\cdot\mathbf{n}\,\mathrm{d}\sigma + (\rho_p^{(i)} - \rho_f)\,V_p^{(i)}\,\mathbf{g}$$
$$I_p^{(i)}\,\dot{\boldsymbol{\omega}}_p^{(i)} = \rho_f \oint_{\partial\mathcal{S}^{(i)}} \mathbf{r}\times(\boldsymbol{\tau}\cdot\mathbf{n})\,\mathrm{d}\sigma$$

MOAT – project timeline

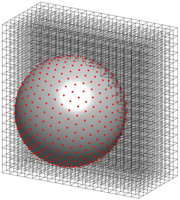


- first phase: uncoupled simulations of particle-bound and dissolved bacteria

→ series of small-scale simulations on ForHLR II (8.5 mio / 15 mio CPU hours)

- second phase: single large-scale simulation of coupled system (probably on Hazel Hen, ∼ 40 mio CPU hours)

Numerical methodology – particles



Immersed boundary method (IBM)

Uhlmann, 2005

- finite-difference DNS on fixed Cartesian grid, uniform
- rigid body motion is imposed by additional body force in momentum equations

Discrete element method (DEM)

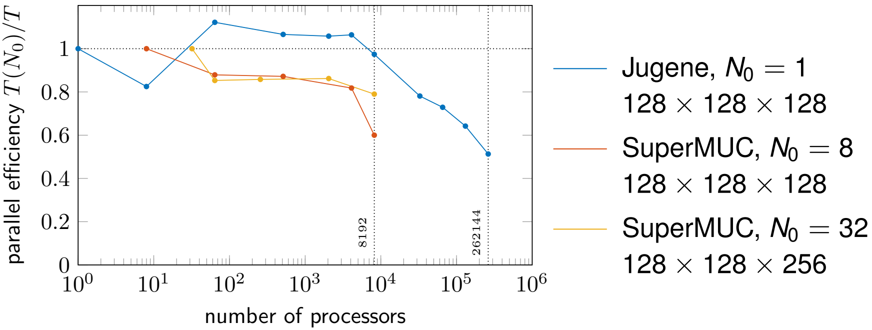
Kidanemariam & Uhlmann, 2014

- realistic particle collisions using spring-damper model

Challenges

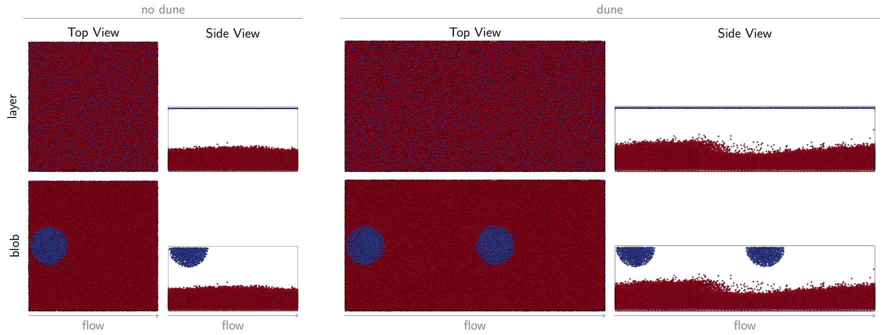
- large number of particles $\mathcal{O}(10^5..10^6)$
- particles have finite-size and thus might affect multiple parts of decomposed fluid domain

Weak scaling – IBM code



- scales very well in our region of interest
- scaling at HLRS yet to be done (test account granted)

First phase: particle-bound MOs



- first phase: investigate sensitivity to different initial conditions
- influence of initial contaminant distribution, bedforms, particle density

→ gather information on how to set up large scale simulation

UV inactivation of particle-bound MOs

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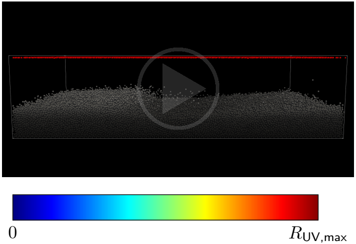


$$Re_b = 3000, \quad \text{dunes}, \quad \text{layer},$$

$$Ga_c = 20, \qquad Ga_s = 28,$$

$$\rho_c^* = 1.75, \qquad \rho_s^* = 2.5,$$

$$N_{p,c} = 2000, \qquad N_{p,s} = 127070$$

$$N_{\mathrm{proc}} = 288 \qquad t_{\mathrm{cpu}} \approx 250000\mathrm{h}$$

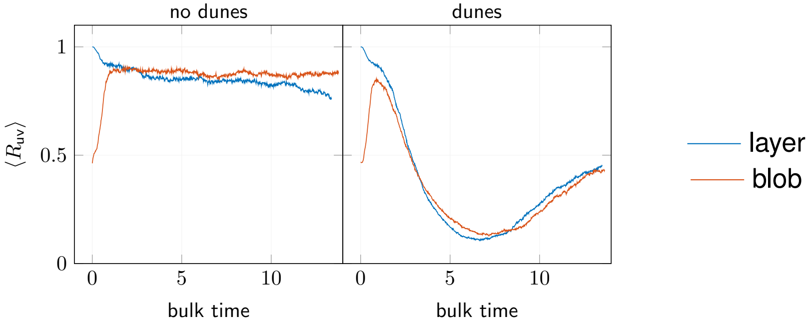
UV inactivation rate in engineering-type models

$$R_{\mathrm{uv}}^{(i)}(t) = \alpha I_{\mathrm{uv},0}\, \exp(-k_{\mathrm{att}}(\Phi_p)\, z^{(i)}(t))$$

UV inactivation rate adapted to inhomogeneities

$$R_{\mathrm{uv}}^{(i)}(t) = \alpha I_{\mathrm{uv}}(\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N_p)}, t)\, \exp(-k_{\mathrm{att}}\, z^{(i)}(t))$$

UV inactivation of particle-bound MOs



- UV inactivation is clearly influenced by presence of dunes and their dynamics

→ completely neglected by engineering-type models

- influence of initial contaminant distribution is rather small

Summary

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Impact on water technology

- flow inhomogeneities and morphodynamics clearly affect fate of bacteria

$\rightarrow$ quantification of those effects can be used directly to improve simpler models

- ability to study small-scale behavior which is not easily accessible by simple models or experiment

Computational challenges

- multi-scale problem (turbulence, low diffusivity mixing)
- large number of moving solid-fluid interfaces (particles)

Thank you for your attention

Feel free to ask questions!

References I

[1] M. Uhlmann, ”An immersed boundary method with direct forcing for the simulation of particulate flows”, Journal of Computational Physics, Bd. 209, Nr. 2, S. 448-476, 2005.

[2] A. G. Kidanemariam und M. Uhlmann, ”Interface-resolved direct numerical simulation of the erosion of a sediment bed sheared by laminar channel flow”, International Journal of Multiphase Flow, Bd. 67, S. 174-188, 2014.