Emulation of an individual-based model simulation of microbial communities

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http://research.ncl.ac.uk/nufeb

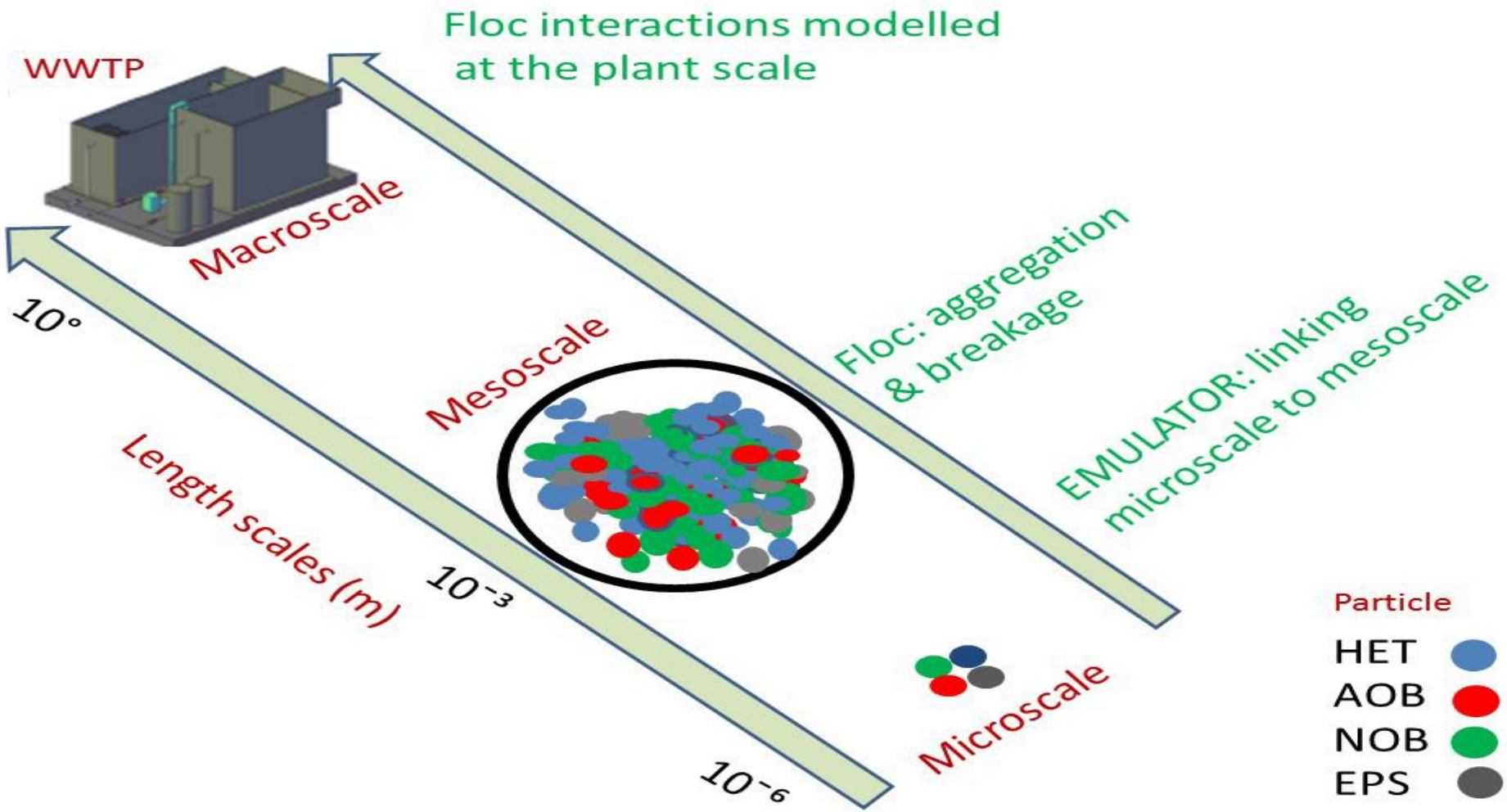
Introduction

- Wastewater treatment plants are open systems that depend on many species of bacteria
- Methods that require many simulator runs become impractical if a single simulator run at one input value takes a long time
- The influence of hydrodynamic shear force on biofilm deformation
- Outputs: number of shear events, volume of detached cluster

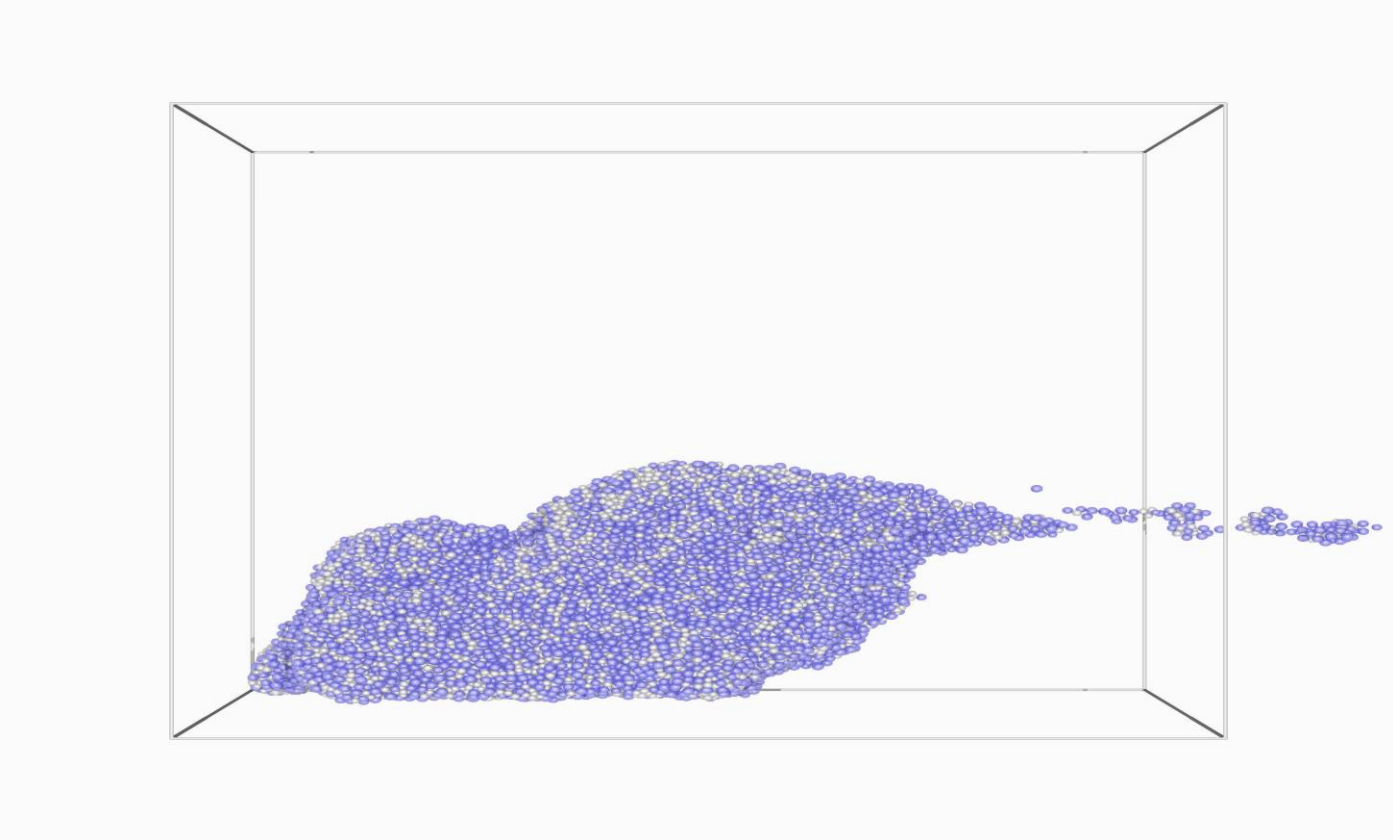
Inputs: biofilm height, surface roughness, mass and EPS composition

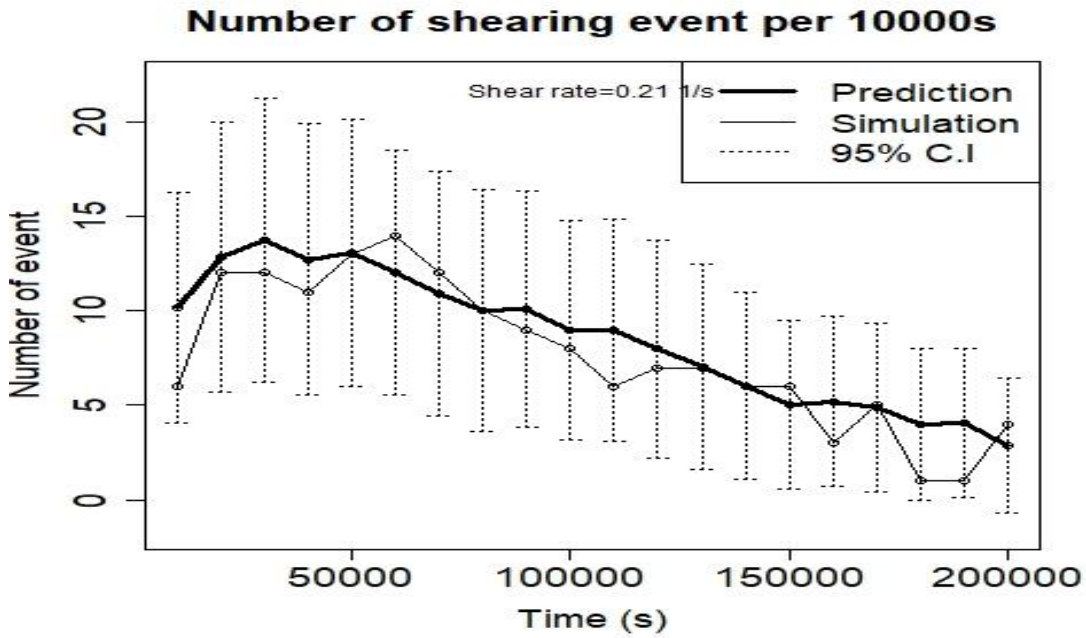
- Bayesian Poisson regression and dynamic linear models (DLMs)

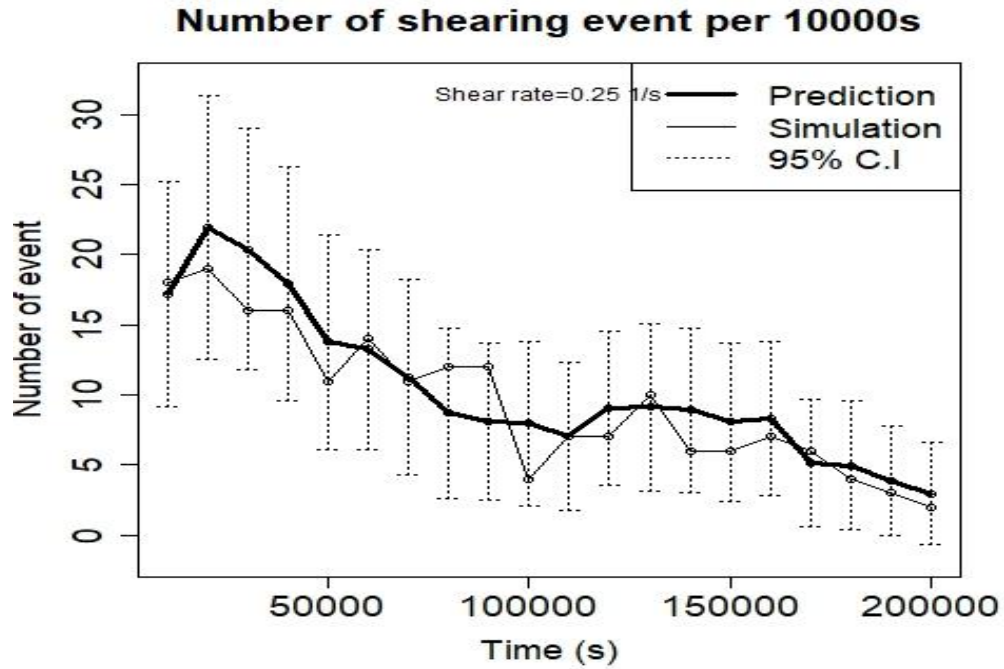
The problem

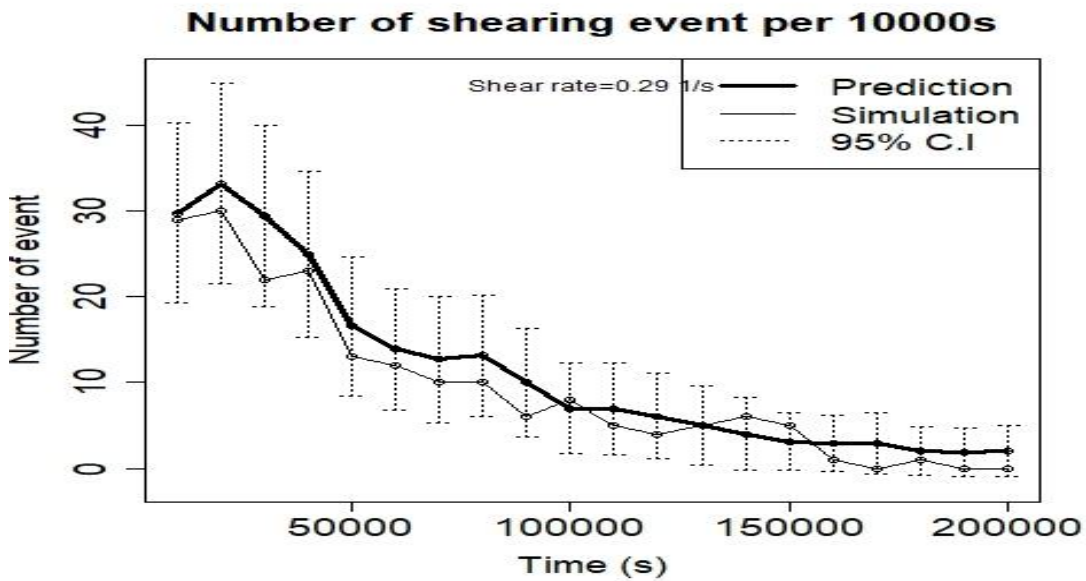

Floc interactions modelled at the plant scale
WWTP
Macroscale
Mesoscale
Microscale
Floc: aggregation & breakage
EMULATOR: linking microscale to mesoscale
Length scales (m)
10°
10⁻³
10⁻⁶
Particle
HET
AOB
NOB
EPS

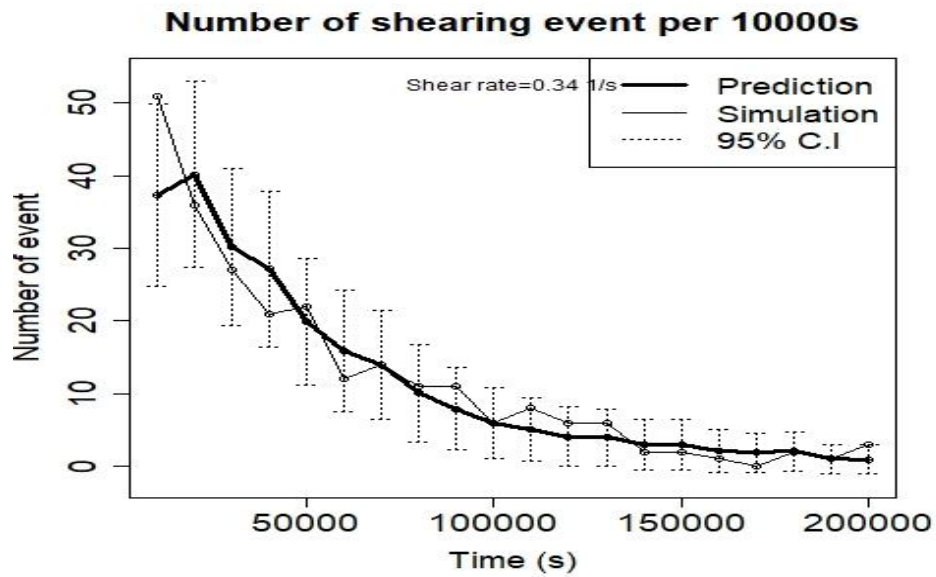
Biofilm simulation under flow fields




Number of shearing event per 10000s
Shear rate=0.21 1/s
Prediction
Simulation
95% C.I
Number of event
Time (s)
0
5
10
15
20
50000
100000
150000
200000


Number of shearing event per 10000s
Shear rate=0.25 1/s
Prediction
Simulation
95% C.I
Number of event
Time (s)
0
5
10
15
20
25
30
50000
100000
150000
200000


Number of shearing event per 10000s
Shear rate=0.29 1/s
Prediction
Simulation
95% C.I
Number of event
Time (s)
0
10
20
30
40
50000
100000
150000
200000


Number of shearing event per 10000s
Shear rate=0.34 1/s
Prediction
Simulation
95% C.I
Number of event
Time (s)
0
10
20
30
40
50
50000
100000
150000
200000

Summary

- Evaluate the strategy for emulating high-level summary from the individual-based simulation of microbial communities using the NUFEB 1.1
- Measure aggregated characteristics on the microscale simulation
- Apply a dynamic Bayesian surrogate model (GP emulator) for modelling the interesting morphological characteristics that are essential for the design and performance of wastewater reactor.
- Perform Bayesian sensitivity analysis to identify the most influential input parameters.
- Quantify and model detachment patterns of a biofilm in response to hydrodynamic shear stress.

Future plans

We have made considerable progress on the parameter calibration using the recently released **NUFEB 2.0** version of the model

- ❖ Continue with the NUFEB 2.0 parameter calibration using IdynoMICS and experimental data.
- ❖ Plan to properly investigate the use of emulators as an upscaling strategy to build mesoscale models.