NUFEB

Building an advanced Biological Simulation System using Atomistic Simulation tools

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on behalf of the NUFEB Team

New Horizons in Atomistic Simulation

Friday 5th January 2018

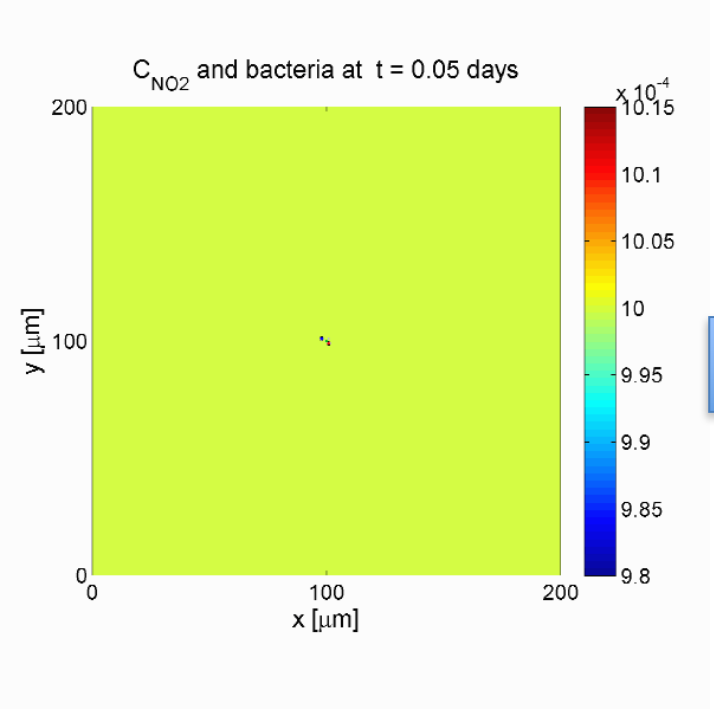
York

Newcastle University

NORTHUMBRIAN WATER living water

nufeb frontiers in engineering biology

Bridging the Gap



NUFEB

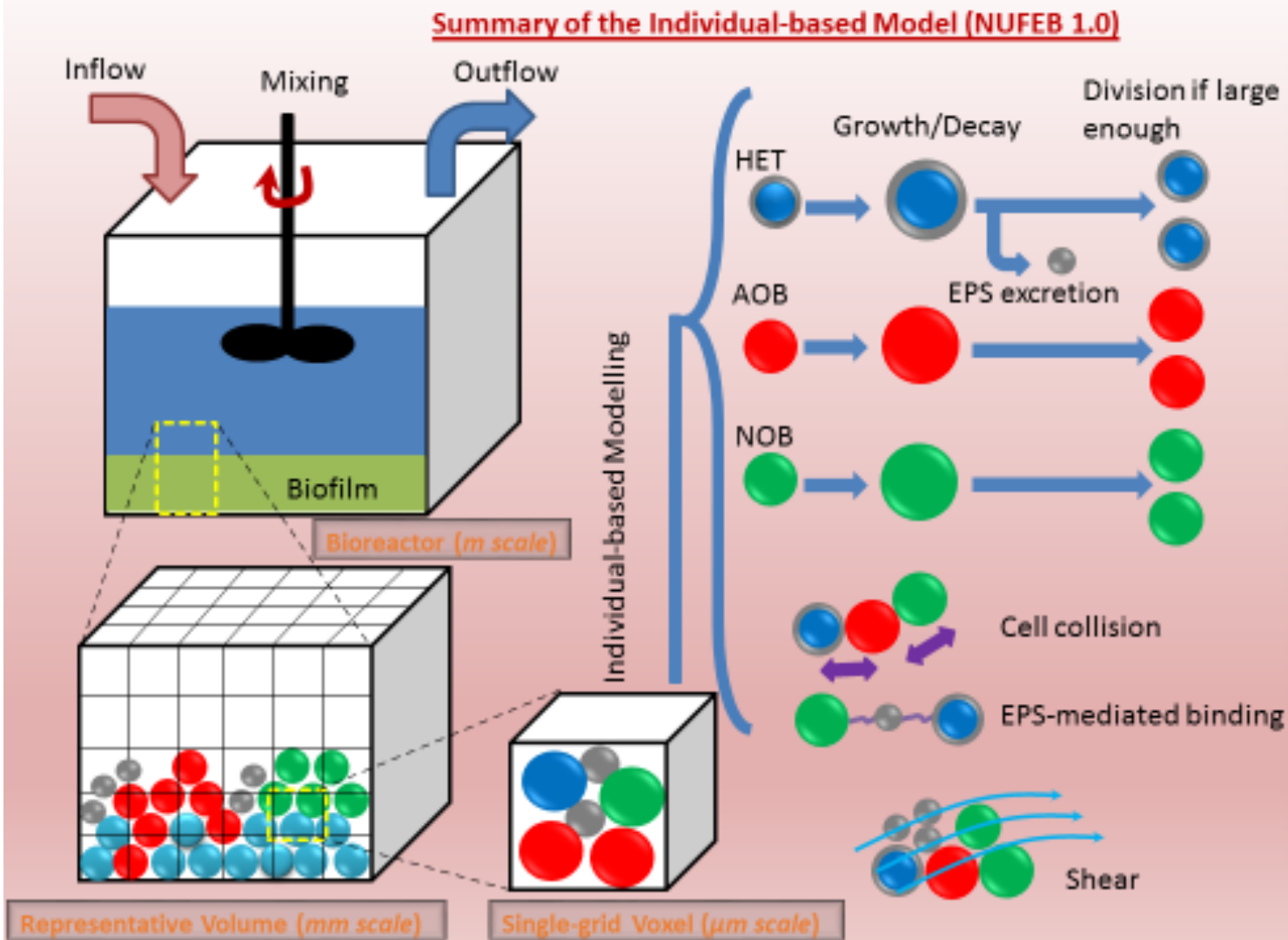
Model Overview

AOB - Ammonia Oxidizer Bacteria

EPS - Extracellular Polymeric Substances

HET - HETerotrophs

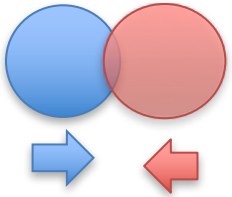
NOB - Nitrite Oxidizer Bacteria



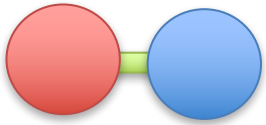
Process Stages

Mechanical Relaxation

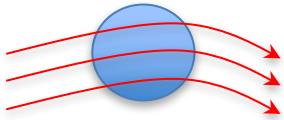
Contact force



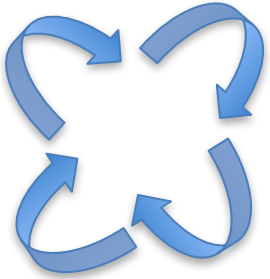
Adhesive force



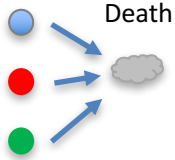
Fluid force

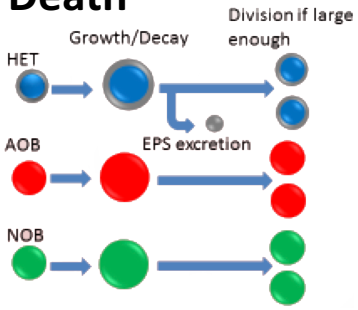


Gravitational force

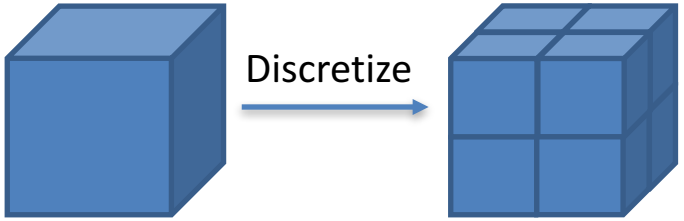


Handle Growth/Decay and Birth / Death



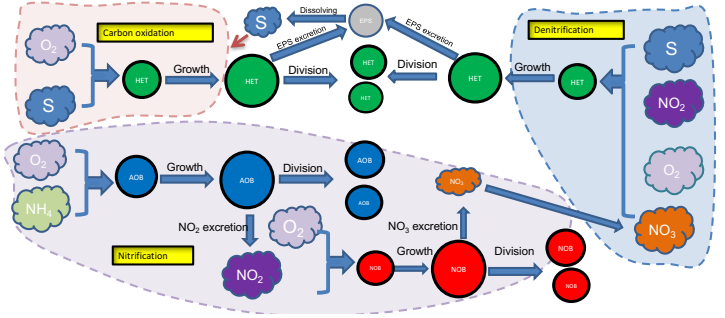


Nutrient Mass Balance



Solve using FDM

Update Growth rates wrt Nutrient



Process Stages

Mechanical Relaxation

Essentially an atomistic simulation system
(Numerous sequential and parallel solvers)

Nutrient Mass Balance

Numerous solvers
(sequential and parallel)

Handle Growth/Decay and Birth / Death

Update Growth rates wrt Nutrient

Bespoke to this problem domain

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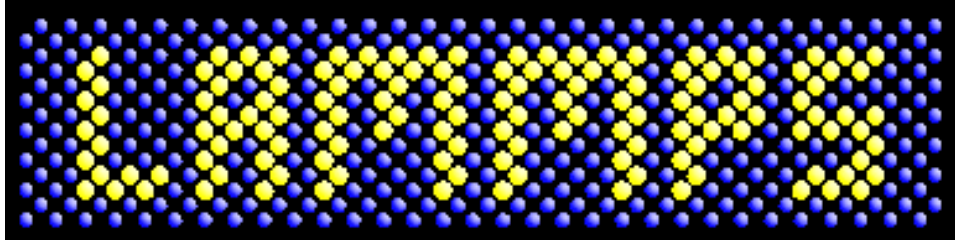
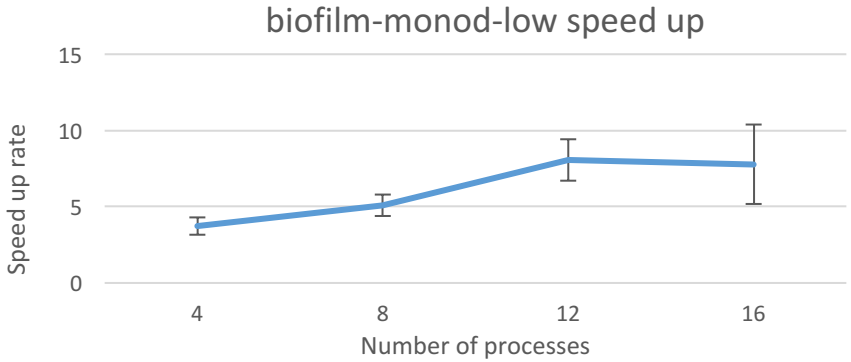
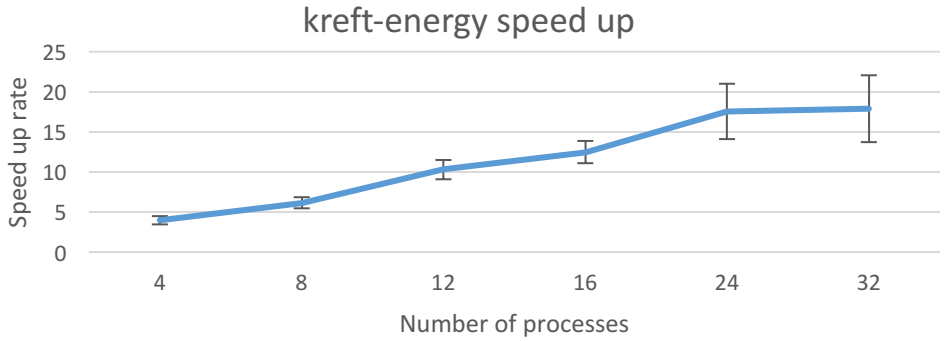
Why LAMMPS?

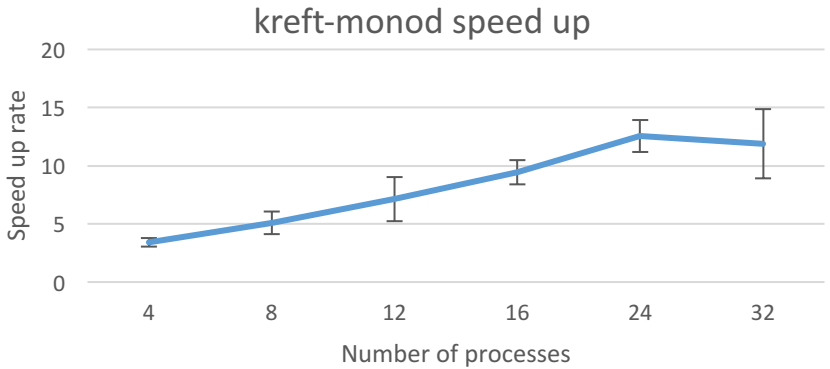


- Mechanical Relaxation considered to be one of the most complex parts of whole solution
- LAMMPS provides:
  - Mechanical processes
  - Has support for FDM
  - Good parallel programming support

Speed-up rates (MPI)







- ~20 times speedup possible (maybe more)
- Need to run larger simulations – current ones are too small to get best improvement
- Different results in parallel case – due to order of calculations and generation of random numbers
- Further investigation needed on this

Load balancing

Summary

- NUFEB 2.0 released
  - Works up to ~10^6 cells
  - Any number of cell types
- Now have extended NUFEB 2.0 to run in parallel
  - OpenMP / MPI
- Future Work
  - Model larger numbers of cells (~10^9)
  - More realistic biology / chemistry / mechanics
- Validation
  - Through experimentation

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Thank you

Newcastle University

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nfeb frontiers in engineering biology