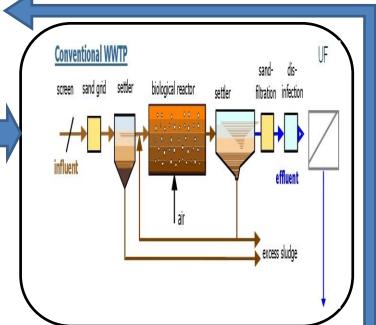
Task 1: Design

Carefully design the experiment to produce a good coverage (LHS)

Task 2: LAMMPS

Run LAMMPS for fixed number of days to obtain microscale simulation data



Task 3: Data Processing

Summarize the relevant outputs from microscale to mesoscale (floc)

Task 4: Emulation

Perform Gaussian process (GP) in form of kriging metamodels

Task 5: Outputs

Emulator provides prediction at mesoscale level