Multiscale Modeling of Membrane Distillation

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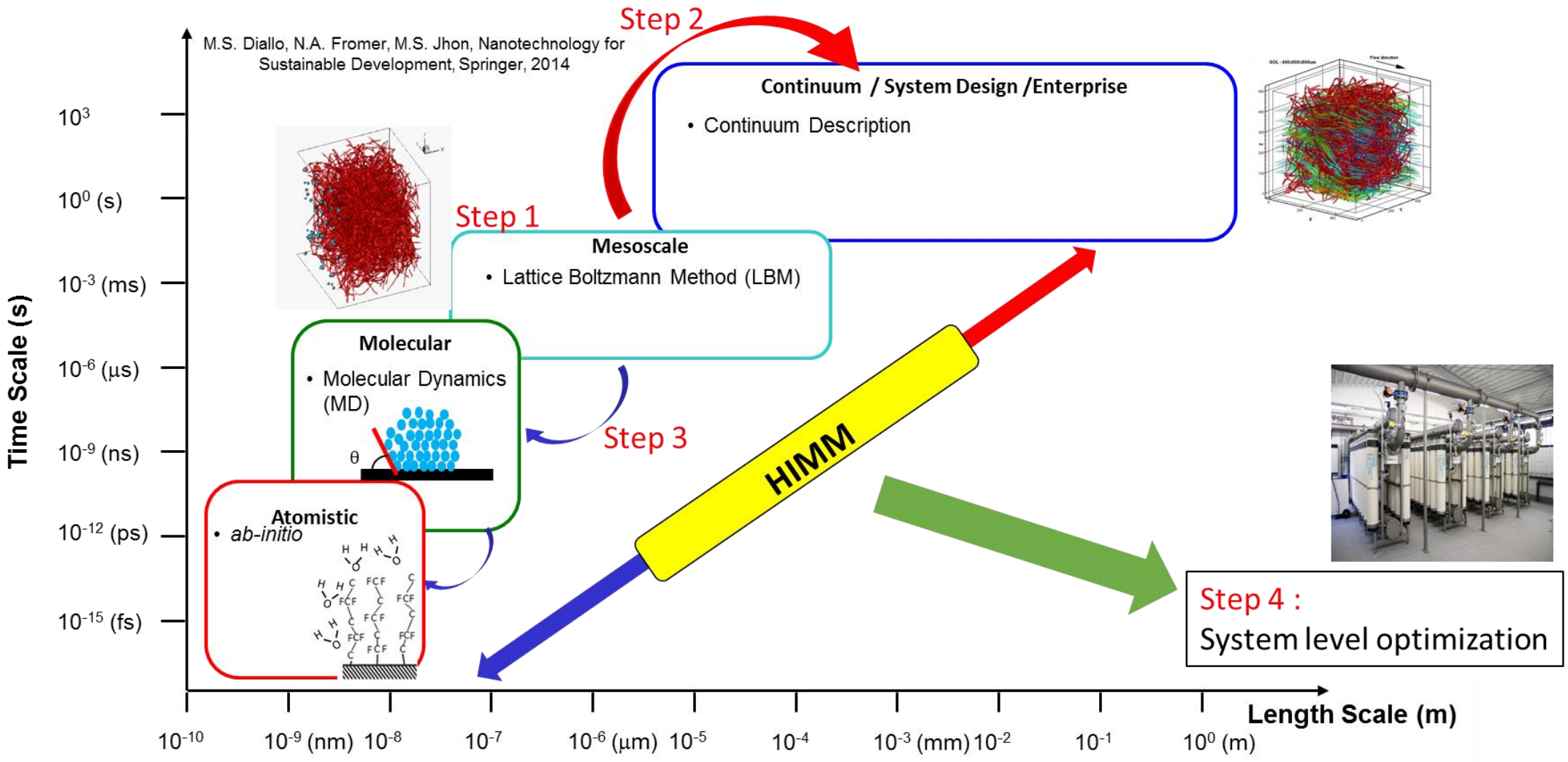
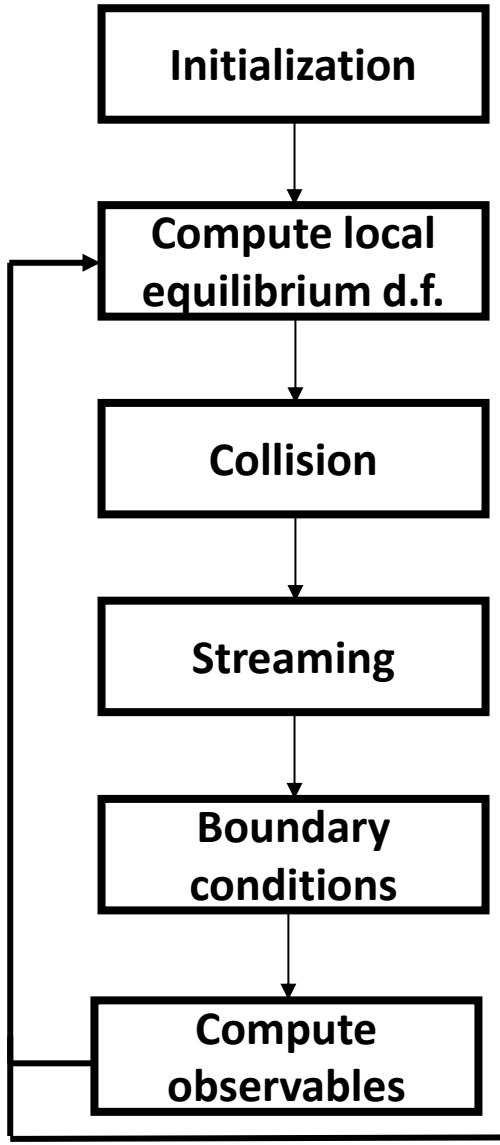
Essence of Multiscale Modeling

Goal: Develop system design criteria via multiscale modeling approach based on Holistic Integrated Multiscale Modeling (HIMM) and optimization (middle-out approach)



Step 1. Lattice Boltzmann Method (LBM) - Centerpiece



$$f_i(\mathbf{x} + \mathbf{e_i}\Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{1}{\tau}\left(f_i(\mathbf{x}, t) - f_i^{eq}(\mathbf{x}, t)\right)$$

Inter-particle force ($\mathbf{F}_{int}$)

$$\mathbf{F}_{int} = -G\psi(\mathbf{x})\sum w_i\psi(\mathbf{x} + \mathbf{e_i})\mathbf{e_i}$$

Adsorption force ($\mathbf{F}_{ads}$)

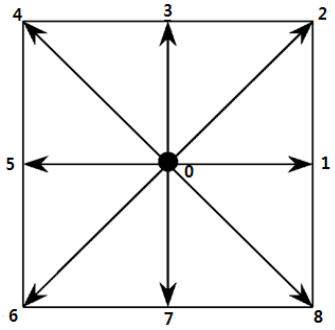
$$\mathbf{F}_{ads} = -G_{ads}\psi(\mathbf{x})\sum w_i\psi(\mathbf{x} + \mathbf{e_i})\mathbf{e_i}$$

@ Equilibrium; $p = \rho c_s^2 + \frac{G}{6}\psi^2$

Shan-Chen (SC) model

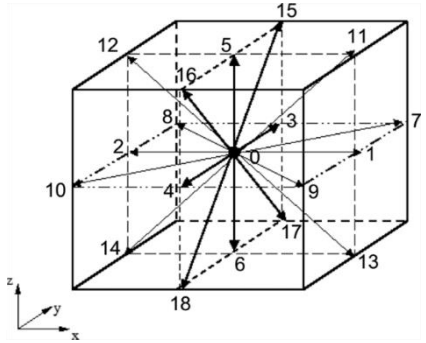
$$\psi(\rho) = \psi_0 \exp\left(-\frac{\rho_0}{\rho}\right)$$

2D



D2Q9
i = 0 - 8

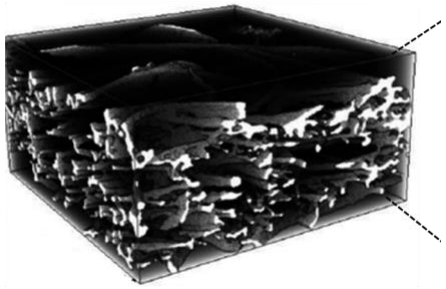
3D



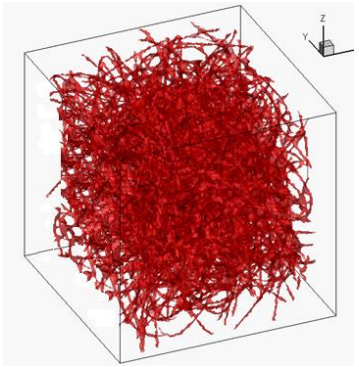
D3Q19
i = 0 - 18

Step 2. Validation of Our LBM Code

XCT image to simulation



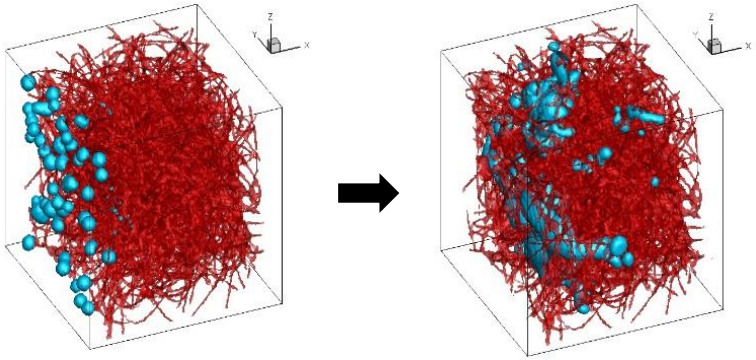
XCT image



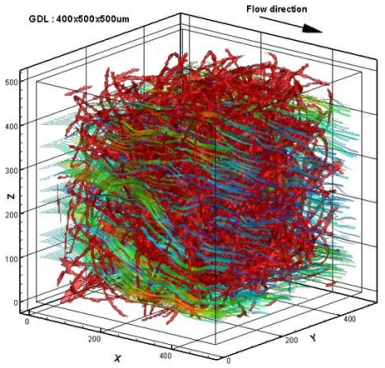
MATLAB generated structure

- By controlling the hydrophobicity, we can calculate contact angles
- Obtain cohesive energy from equation of state
- Obtain adhesive energy from surface-pseudo particle interaction parameter
- Size: 400 X 500 X 500 Lattice units

Results



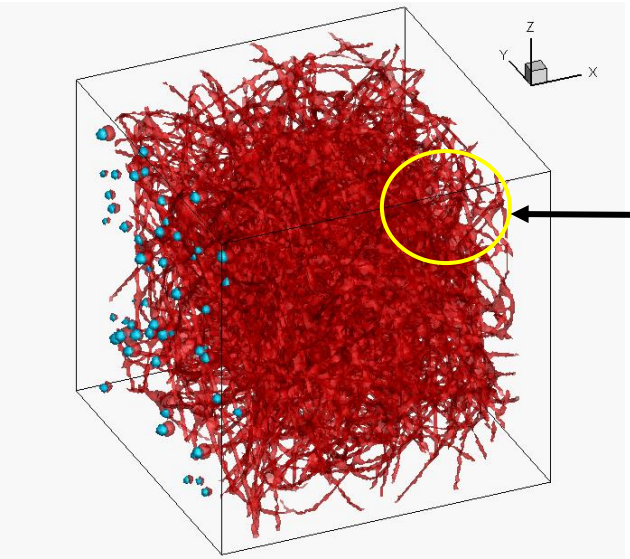
Vapor condenses and flows



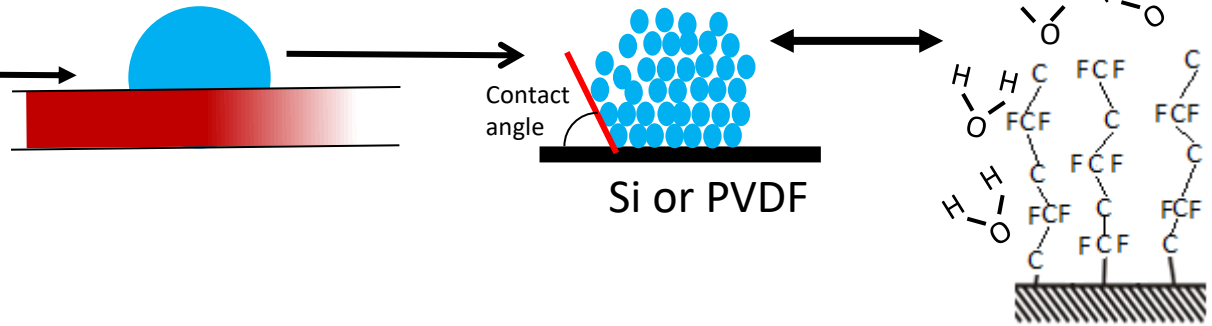
Streamline

Step 3. Linking Mesoscale LBM & Molecular/Atomistic Model

(A) Mesoscale (LBM)



(B) Molecular Dynamics

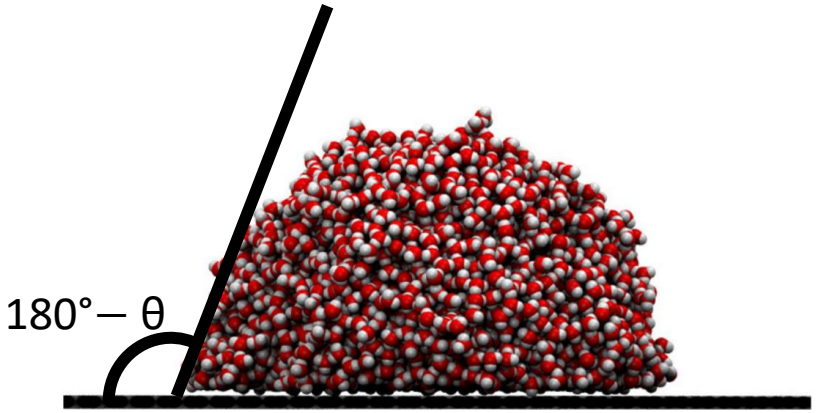


- Need molecular dynamics/Monte Carlo simulation
- Force field analysis based on atomistic scale is required to accurately model potential energy in molecular dynamics
- (A) Mesoscale flow analysis for hydrophobic surface. Water fiber interaction is described by surface-water (pseudo-particle) interaction parameter to analyze contact angle
- (B) Molecular dynamics is performed to calculate contact angle

Step 3 Case Study - Contact Angle Simulation Using MD

Simulation details

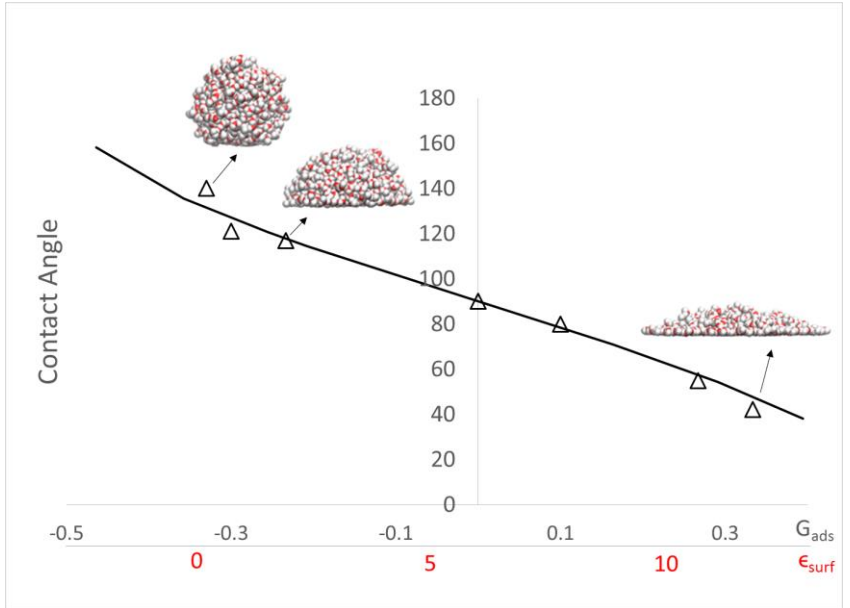
- 800, 1600, 3200, 6400 molecules
- NVT ensemble (Nose-Hoover thermostat)
- Velocity Verlet algorithm (time interval = 10^{-15} s)
- Typical simulation time per data point : 1 week



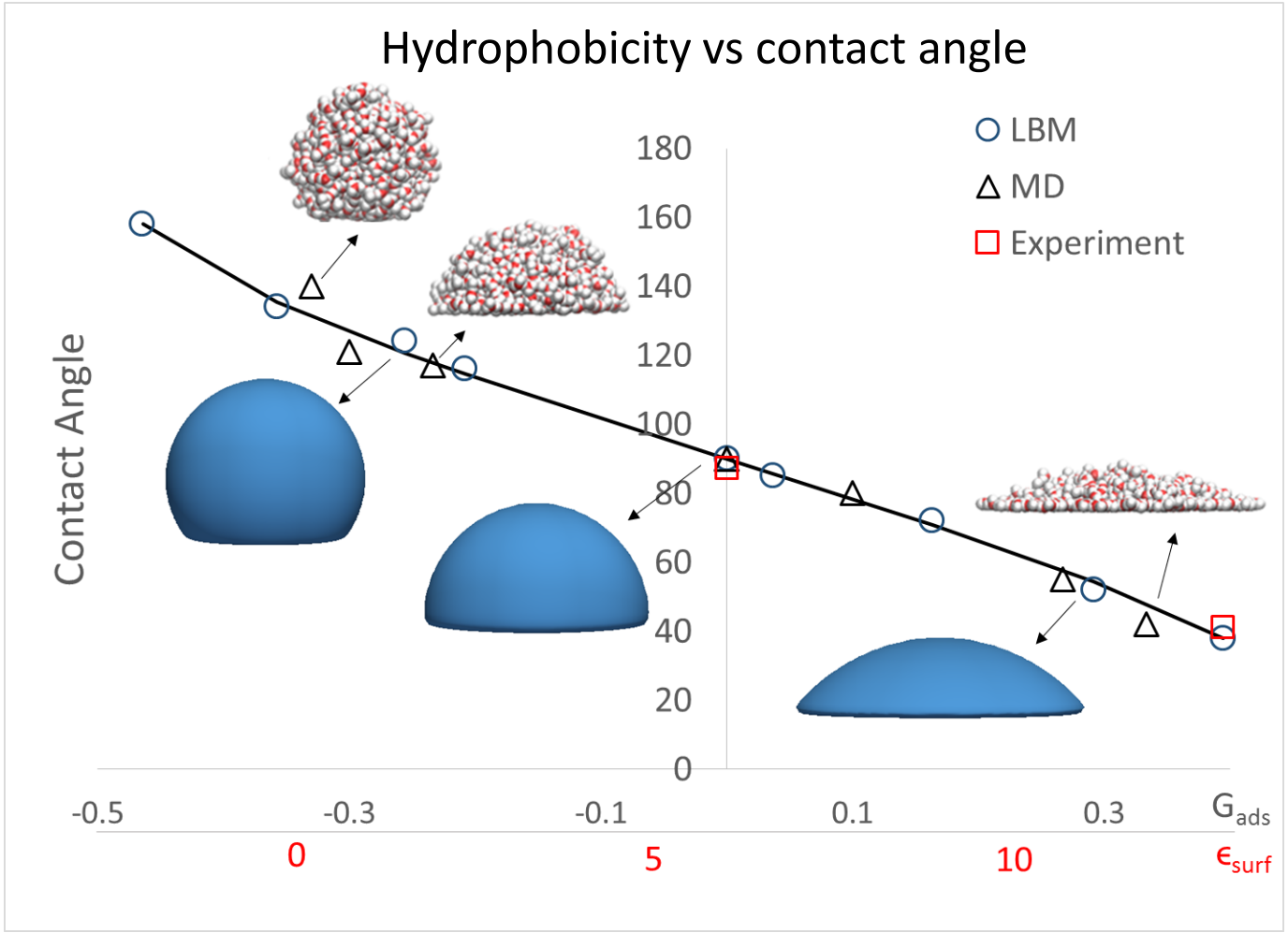
Contact angle : 77° (θ = 103 °)

Parameters	Values
H-O Bond length	1.0 Å
H-O-H Angle	109.47°
Atomic charge : Hydrogen	+0.4238 e
Atomic charge : Oxygen	- 0.8476 e
O-O L-J distance	3.166 Å
O-O L-J energy	0.155 kcal/mol

MD simulation results



Step 3 Case Study Linking Molecular & Mesoscale Simulation



Both LBM and MD calculations are in excellent agreement upon scaling

Simulation results (LBM & MD) and experimental data are in excellent agreement

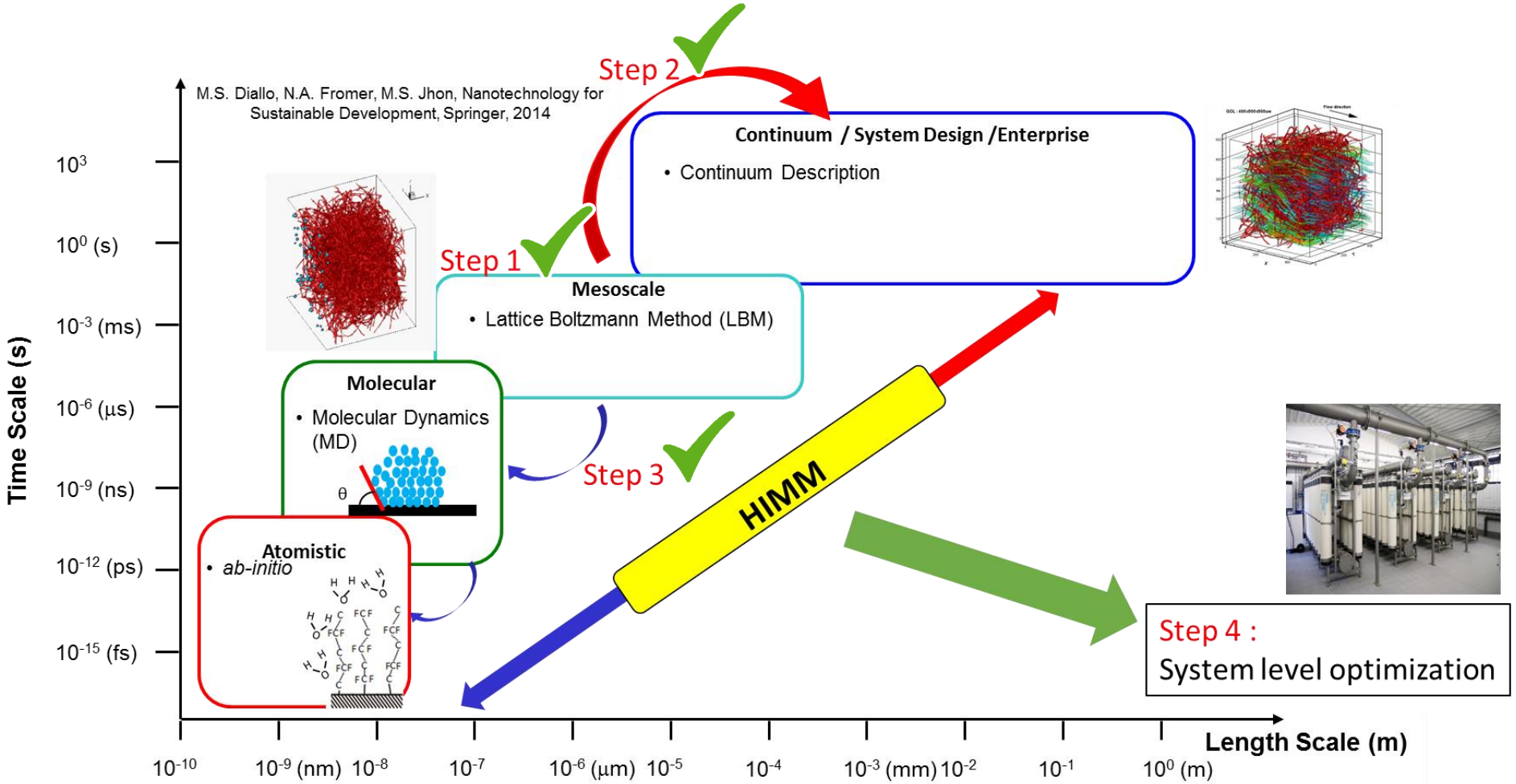
For the first time, we obtained relationship between molecular and mesoscale parameters

LBM MD

$$19.35G_{ads} = \epsilon_{surf} - 6.56$$

Step 4 System Level Optimization

Currently, in progress
Attempts are shown in poster



Conclusion

- We have developed a novel multiscale model, called HIMM, to provide design criteria using molecular/atomistic input using coarse-grained model and reduced order parameters.
- Fuel cell & membrane distillations were chosen as the benchmark examples for HIMM,
- We developed multiphysics LBM code to calculate vapor flux with hydrophobicity as an input. (Step 1&2)
- For the first time, we calculated contact angle using molecular dynamics & LBM (mesoscale analysis) and linked parameters in the both models. (Step 3)
- We are capable of simulating/controlling the vapor flux for molecularly complex surfaces.
- Once multiscale algorithm is fully established, we may be able to provide molecular design criteria for membrane systems. (Step 4)