Simulation Techniques and Scientific Computing
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UNIVERSITÄT SIEGEN

PRACEDAYS'16
Aquatic Purification Assisted by Membranes

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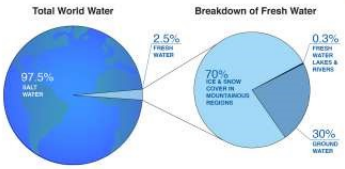
Motivation

- In the 21st Century, supply of mankind with sufficient clean drinking water is a major challange.
- The availability of fresh water is limited.

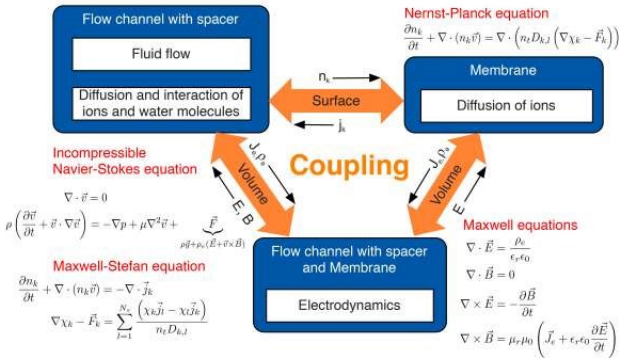


Goal

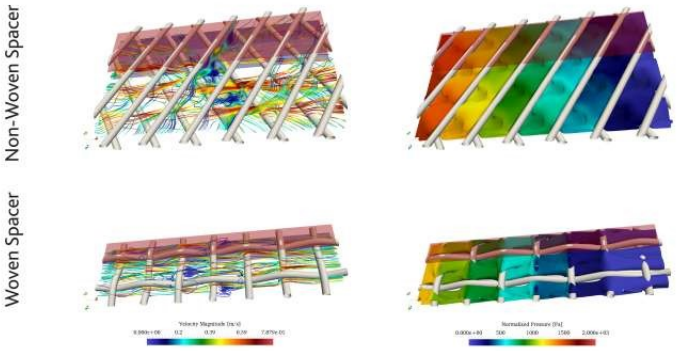
- To understand and optimize the electrodialysis process using high performance computing (HPC).

- M. Johannink, K. Masilamani, A. Mhamdi, S. Roller and W. Marquardt. "Predictive pressure drop models for membrane channels with non-woven and woven spacers". Accepted to Desalination, 2015.
- J. Zudrop, S. Roller, A. Pietro. "Lattice Boltzmann scheme for electrolytes by an extended Maxwell-Stefan approach. Phys. Rev. E 89, 2014.
- J. Zudrop, K. Masilamani, S. Roller, A. Pietro. "A robust lattice Boltzmann method for parallel simulations of multicomponent flows in complex geometries". Submitted to Journal of Computers and Fluids and its under review.

Multi-physical Heterogeneous System



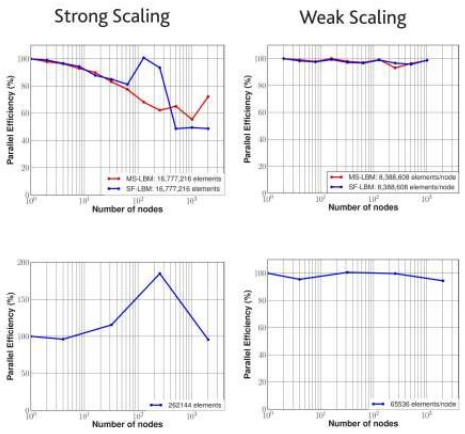
Flow Channel with Spacer



Flow distributions between filaments with stream lines of velocity

Pressure drop across the channel with iso-surface of inflow velocity

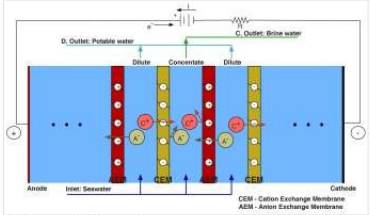
Scalability



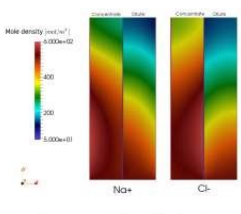
Musubi (LBM solver)
- Periodic domain on HazelHen Cray XC40 system
- Single fluid and Multi-species LBM up to 2048 nodes (49,152 processes)
- Single fluid LBM = 160 FLOP, Multi species LBM = 783 FLOP for 3 species per lattice update

Ateles (Maxwell solver)
- Periodic domain on SuperMUC
- 5th order spatial scheme with Maxwell equations on up to 2048 nodes (32,786 processes)
- 232 x #(degrees of freedom) FLOP for 4th order Runge-Kutta time integration

Electrodialysis Process



Schematic layout



Ions transport in dilluted and concentrated channels

APES framework

- Octree based
- Highly scalable
- End-to-end parallel
- Allows coupling of solvers

Musubi
- Flow channel with spacer geometry

Ateles
- Membrane and electrodynamics

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