TopeSmash

Topology Optimization of Porous Electrodes in Redox Flow Batteries using Scalable Modeling ApproacheS

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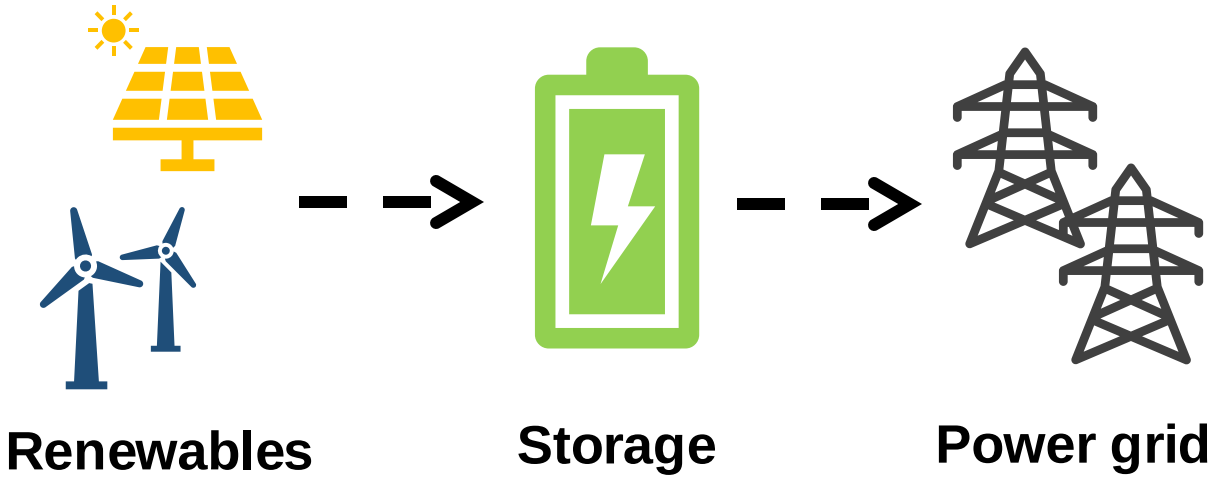
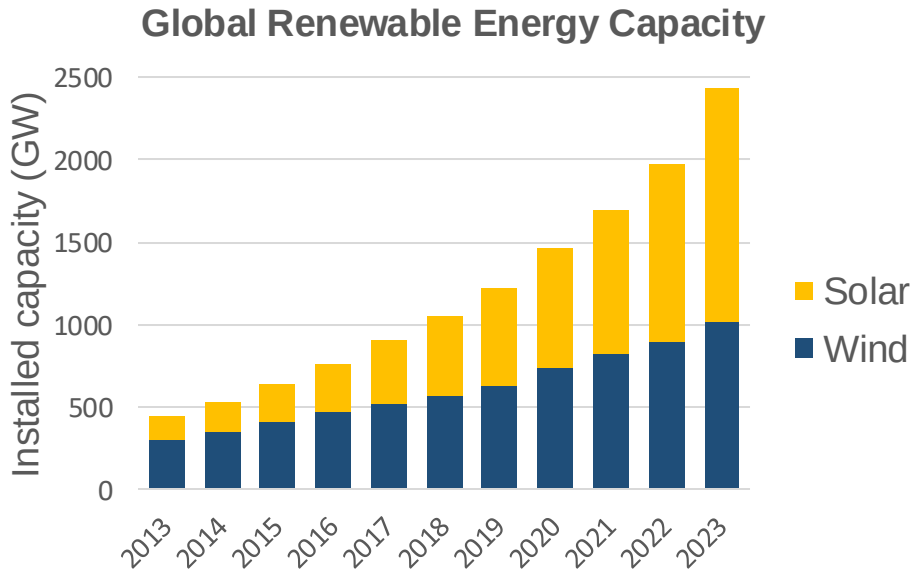
Snellius Advanced User Computing Day 2024
Utrecth, 12th December 2024

Energy Storage

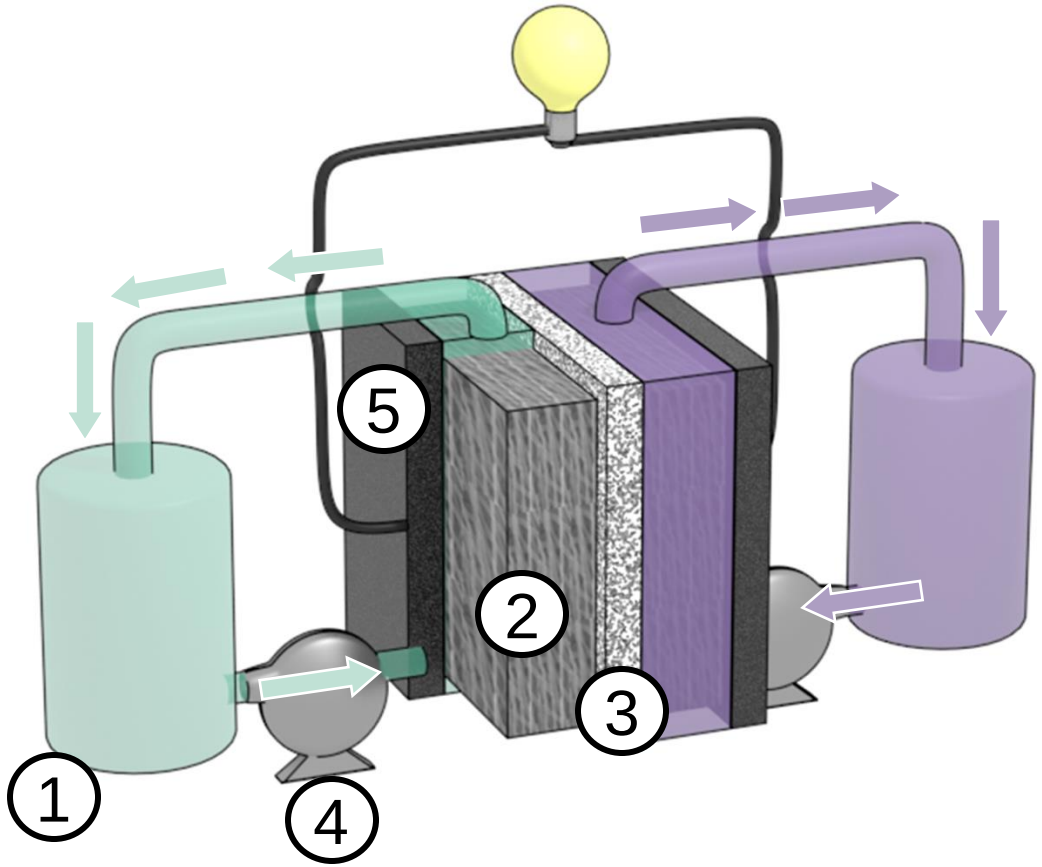
- Renewable energy sources
- Intermittency is an issue





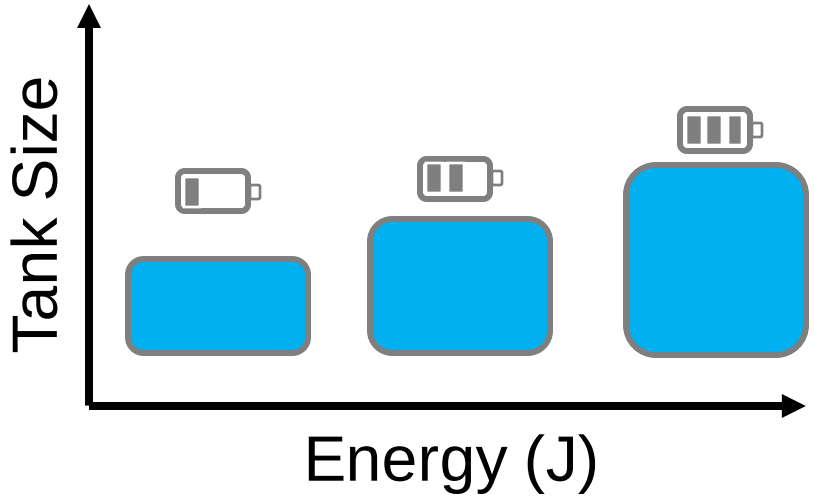
Reuters (2023), International Renewable Energy Agency (IRENA), 2023

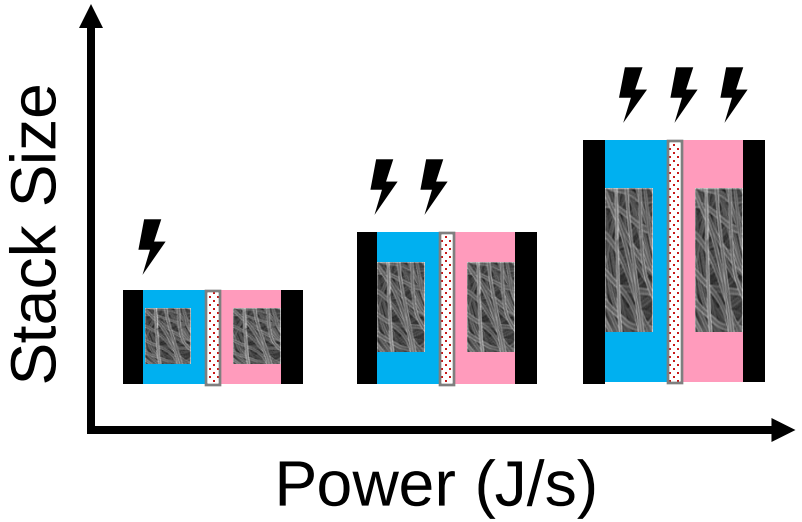
Durable Energy Storage: Redox Flow Batteries (RFB)

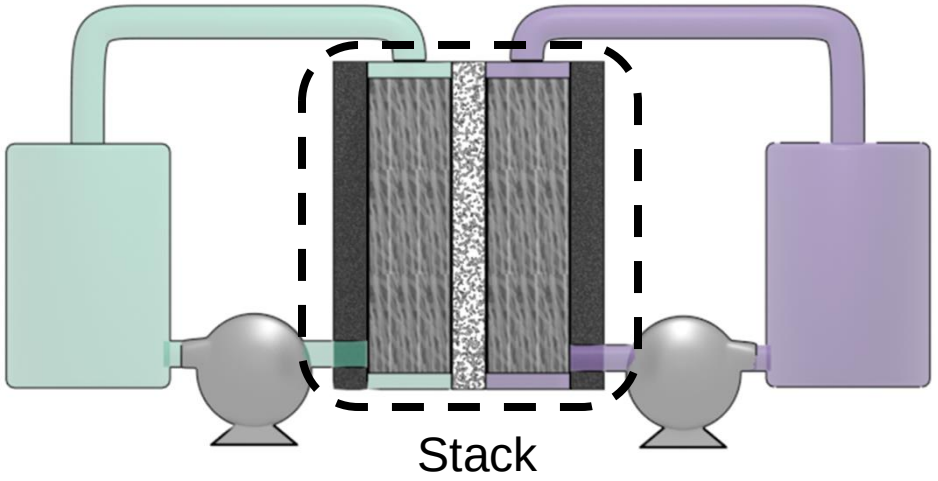


1. Tank
2. Electrode
3. Membrane
4. Pump
5. Current Collector

Decoupled Power & Energy

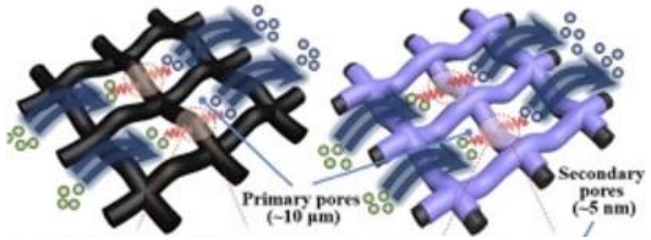


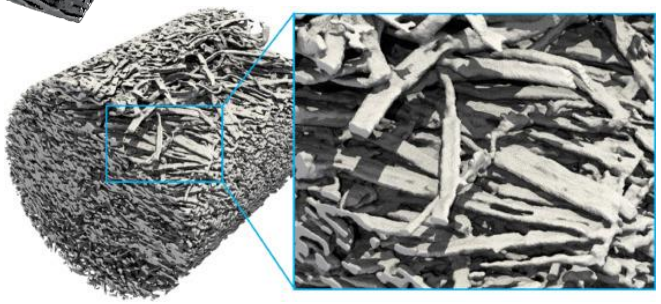


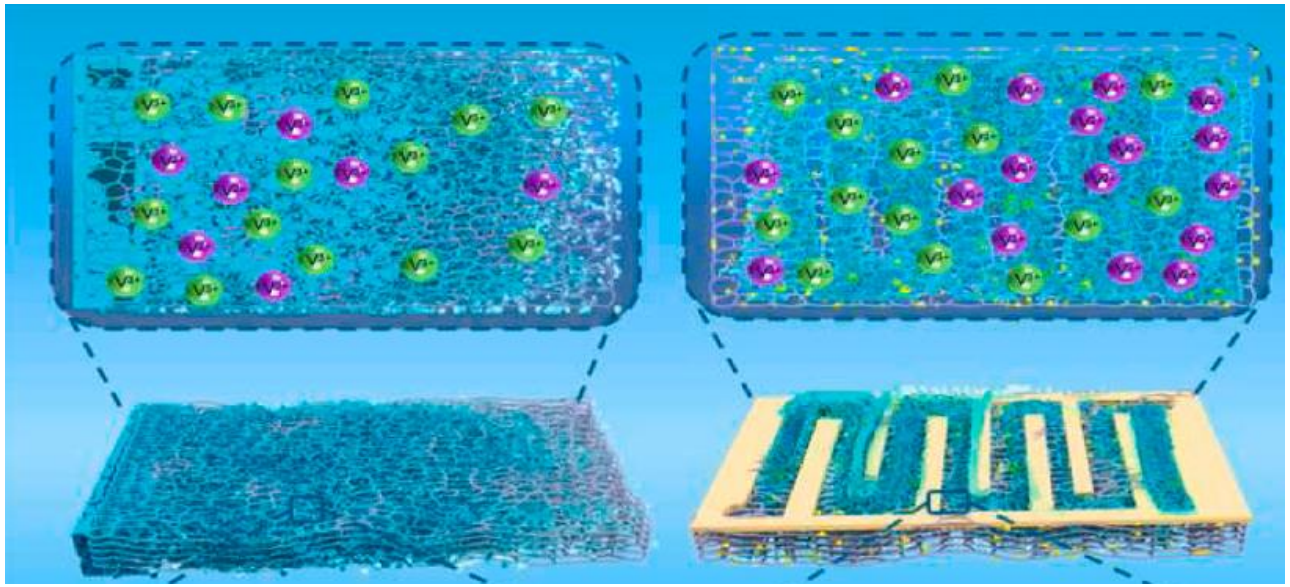


Electrode: Performance-Defining Component

- Where the redox processes occur
- Electrode microstructure & flow field setup govern performance



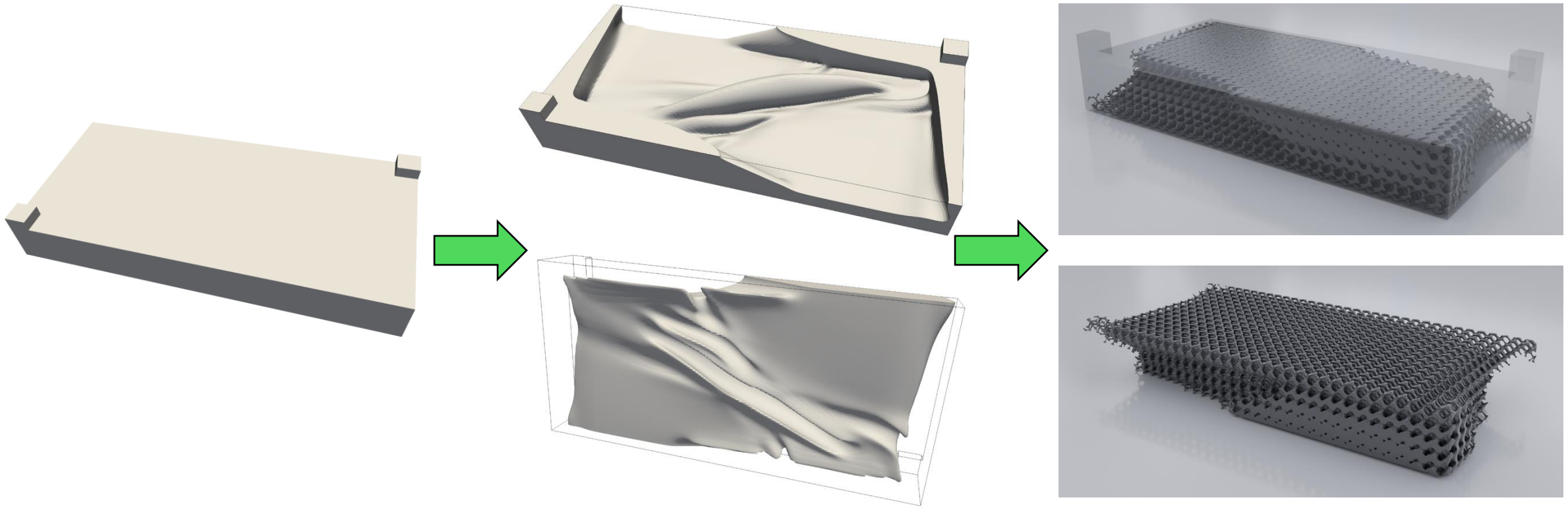




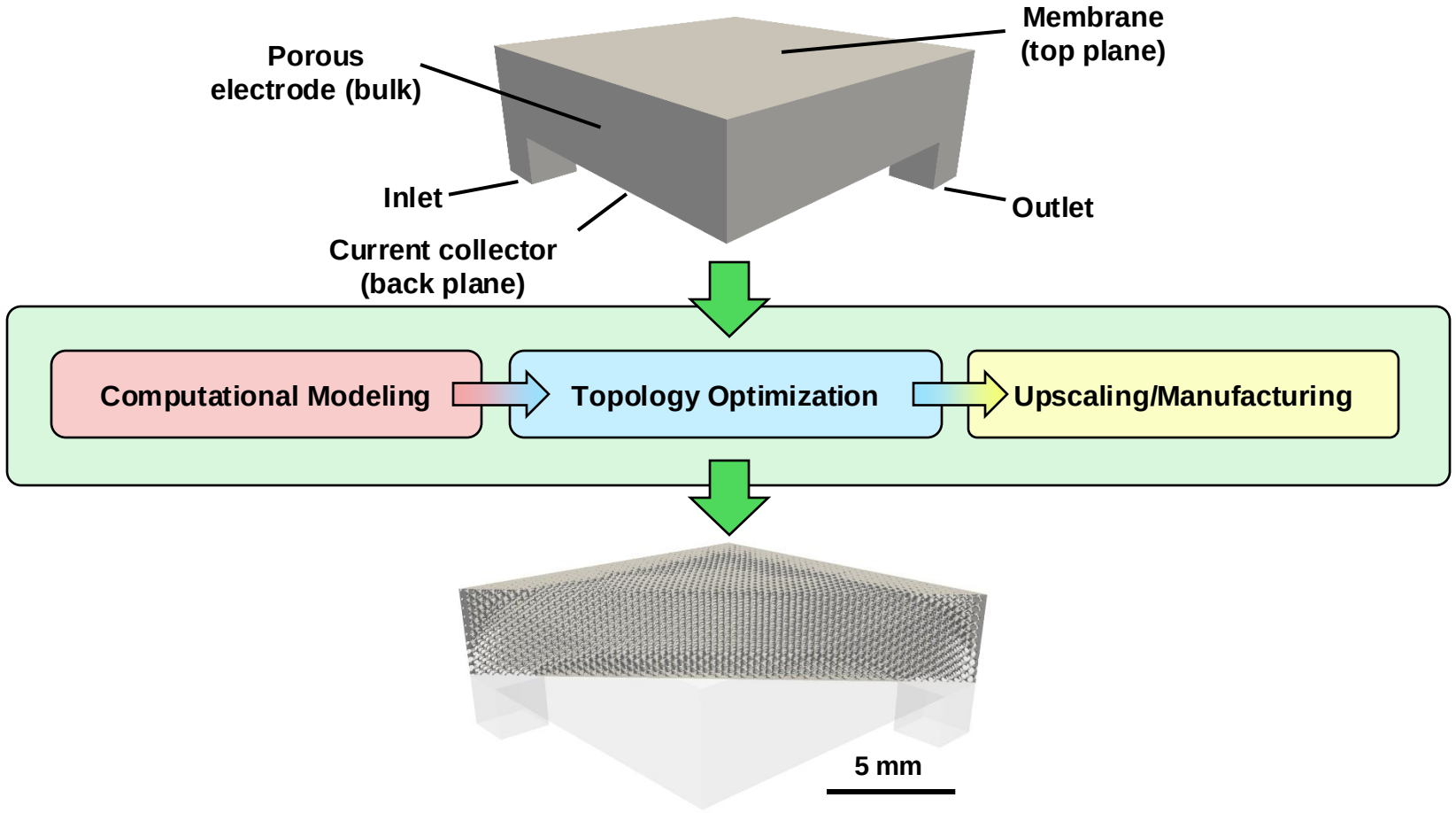
Wan & Jacquemond, Adv. Mater. 33 (2021), Yadav, J. Energy Storage 33, 102079 (2021),
Zhou et al., J. Power Sources., 339 (2017), Cong et al., J. Power Sources., 615 (2024)

Electrode Design via Engineering Optimization?

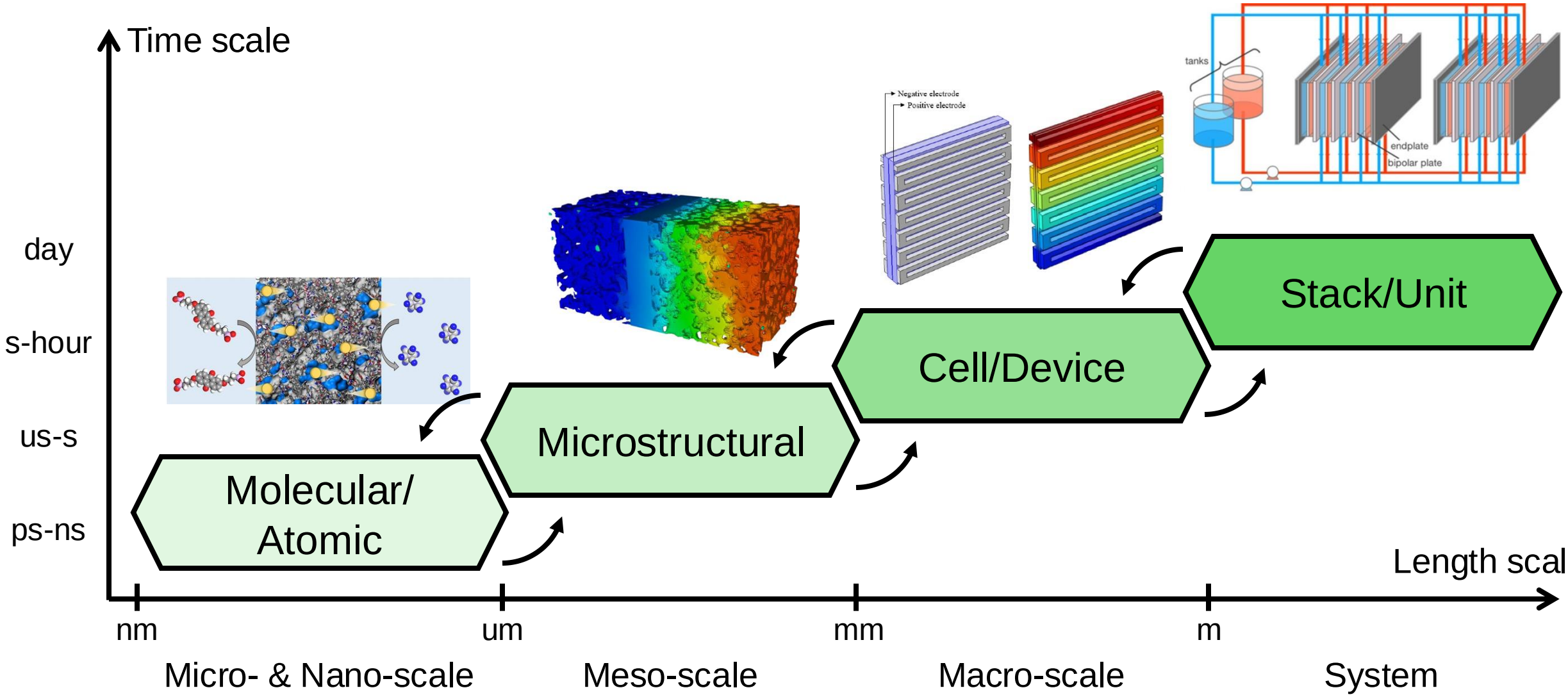
- Inverse design of electrodes for maximizing performance



Modeling Workflow

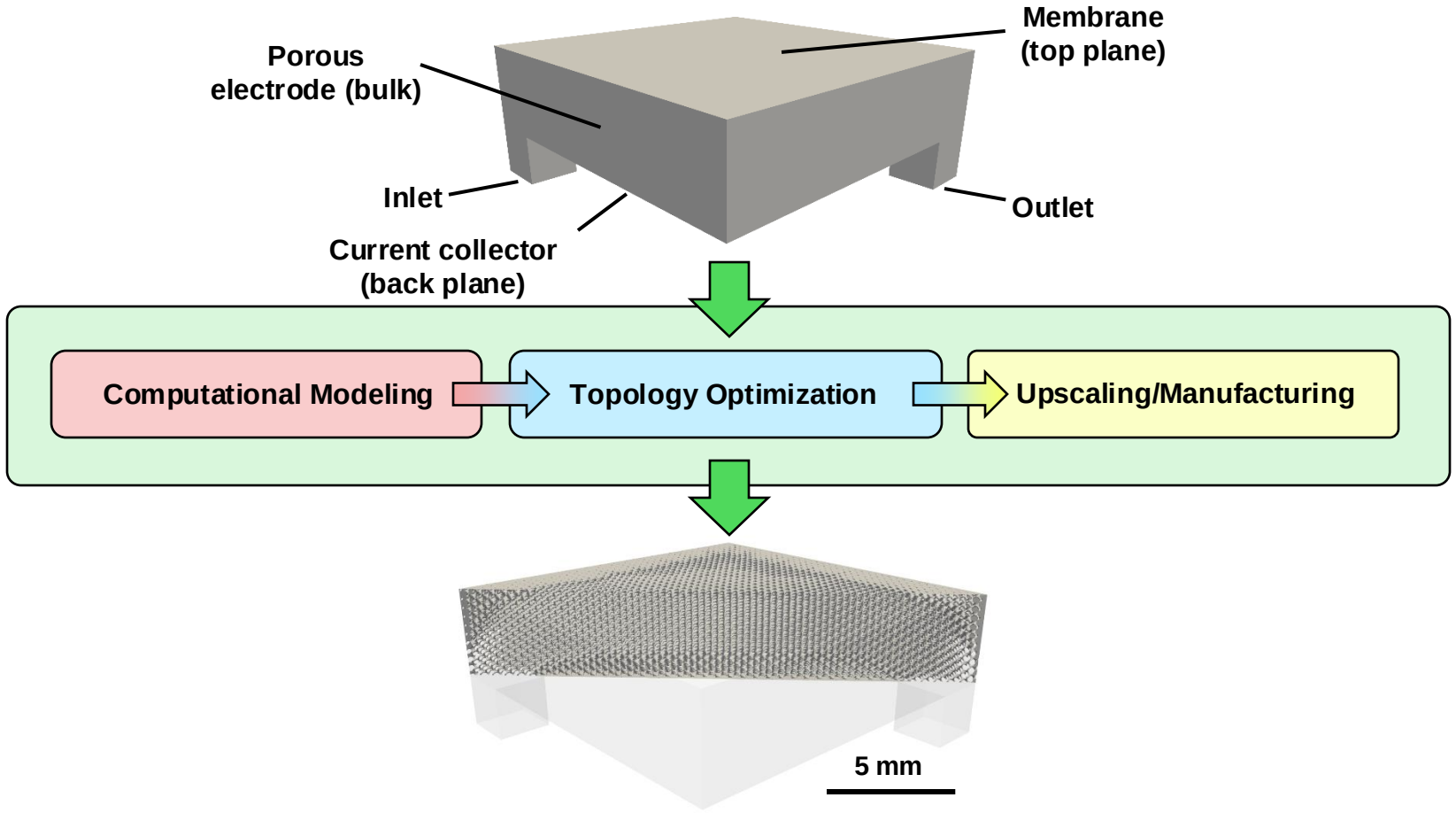


RFBs as Multi-Scale Redox Systems

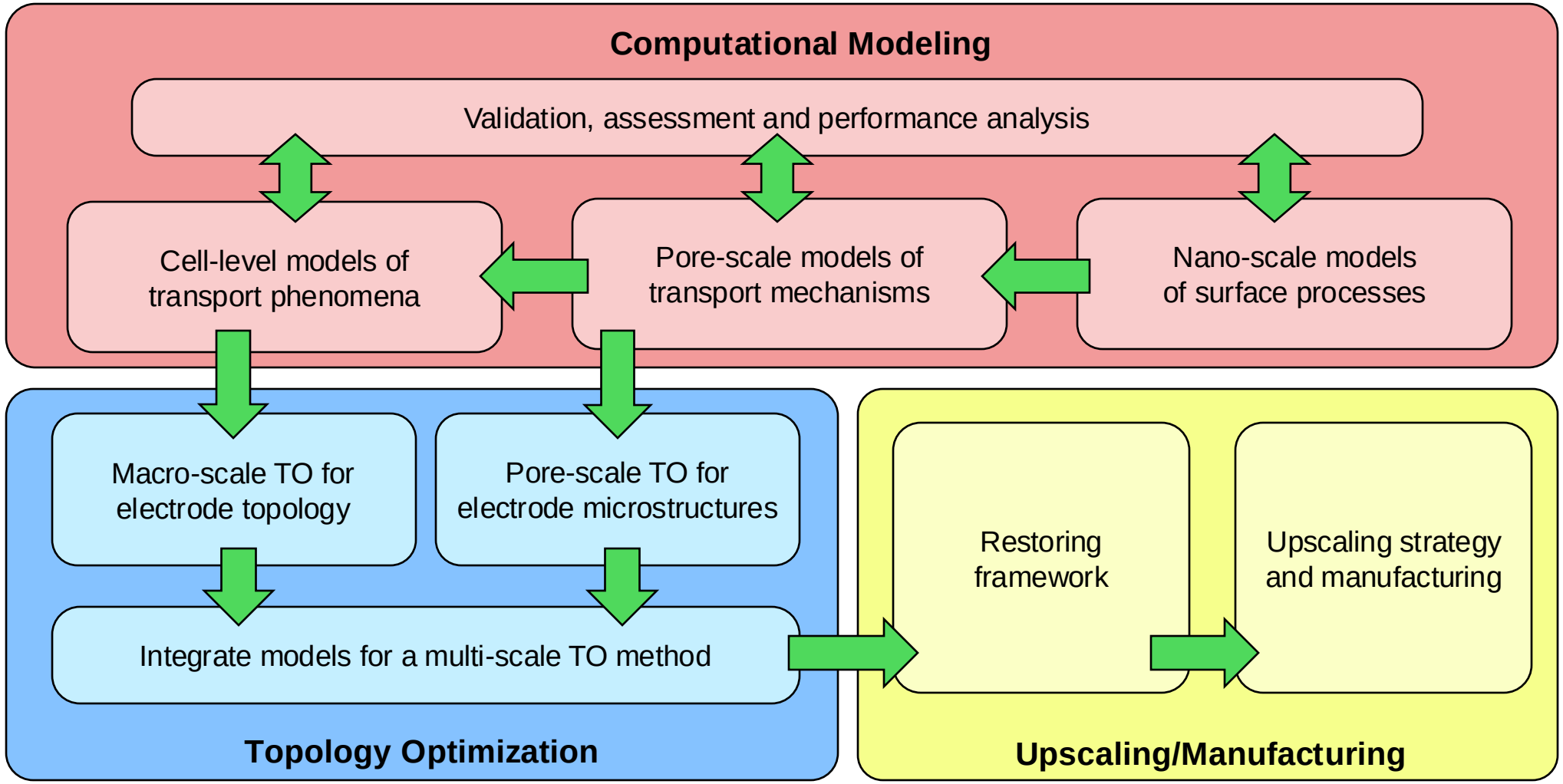


Ye et al., Angew. Chem., 61 (2023) e202207580. De Lauri et al., ACS Appl. Energy Mater., 4 (2021) 13847.
Ali et al., J. Energy Storage, 28 (2020) 101208. Ma et al., J. Electrochem. Soc., 165 (2018) A2209.

Modeling Workflow

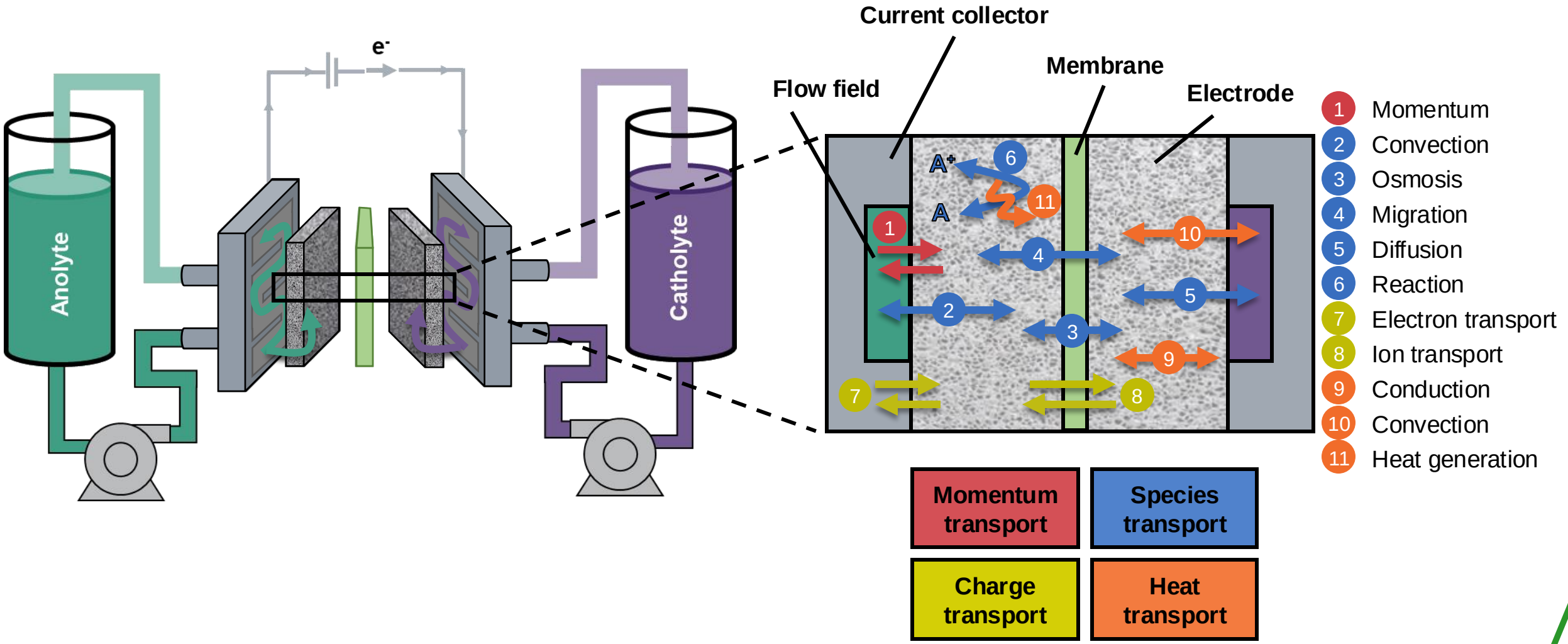


Modeling Workflow

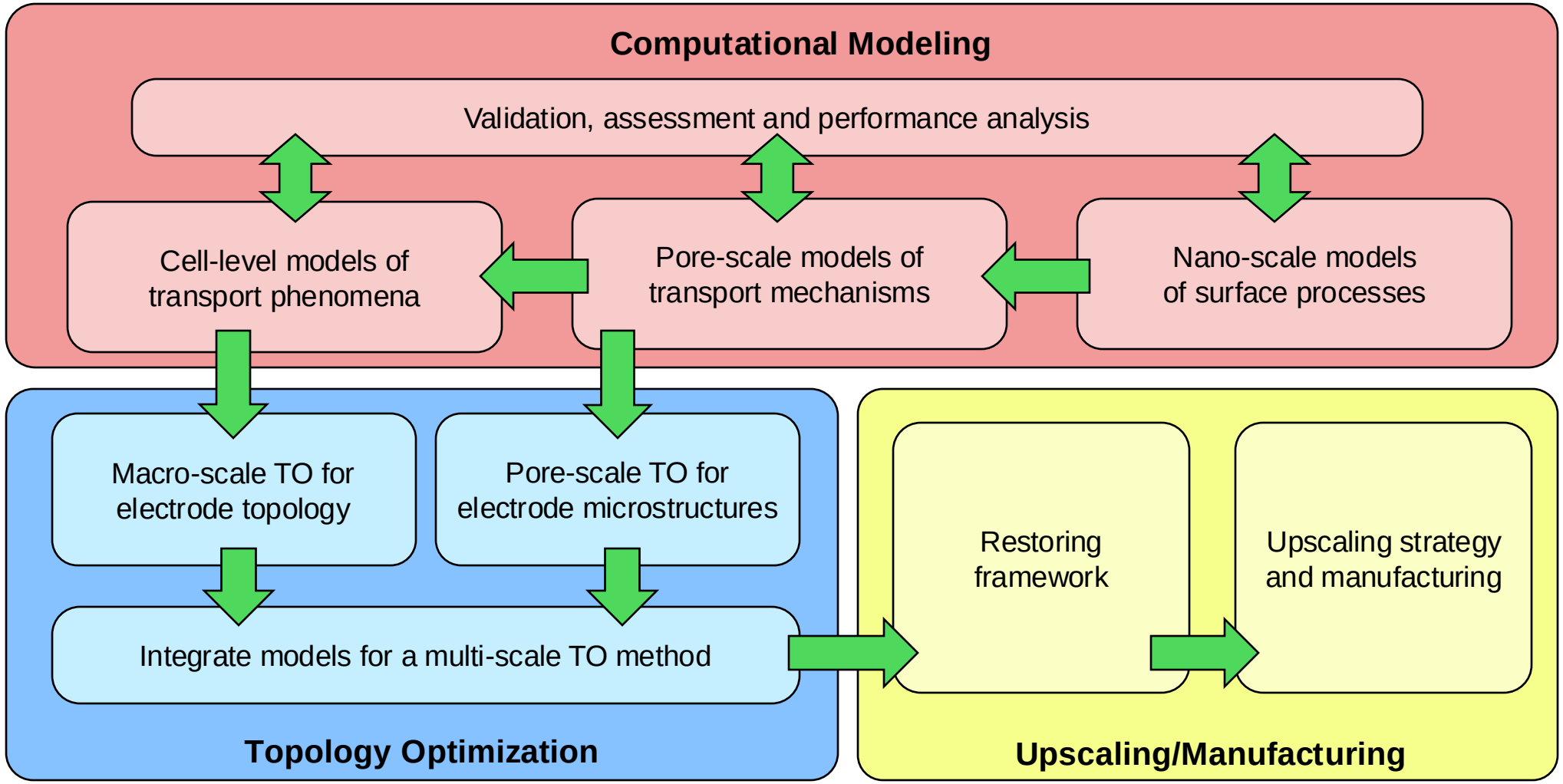


Computational Modeling of RFB Processes

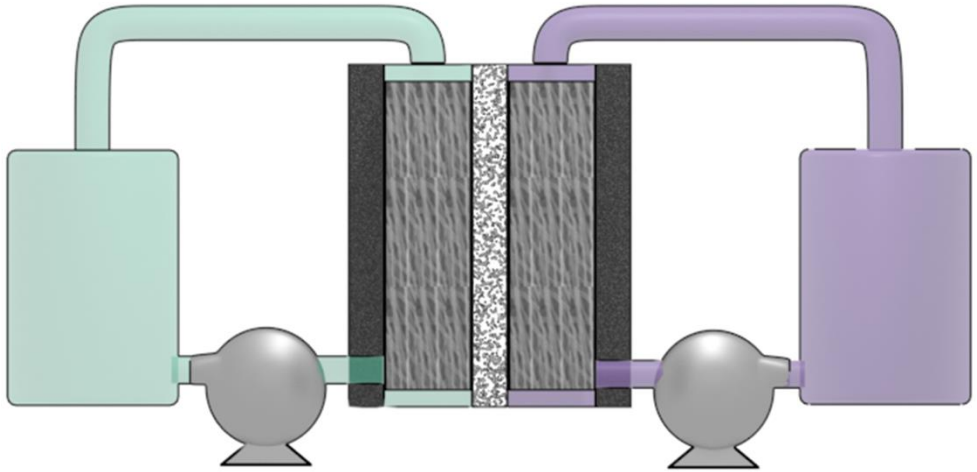
RFBs as Multi-Physics Redox Systems

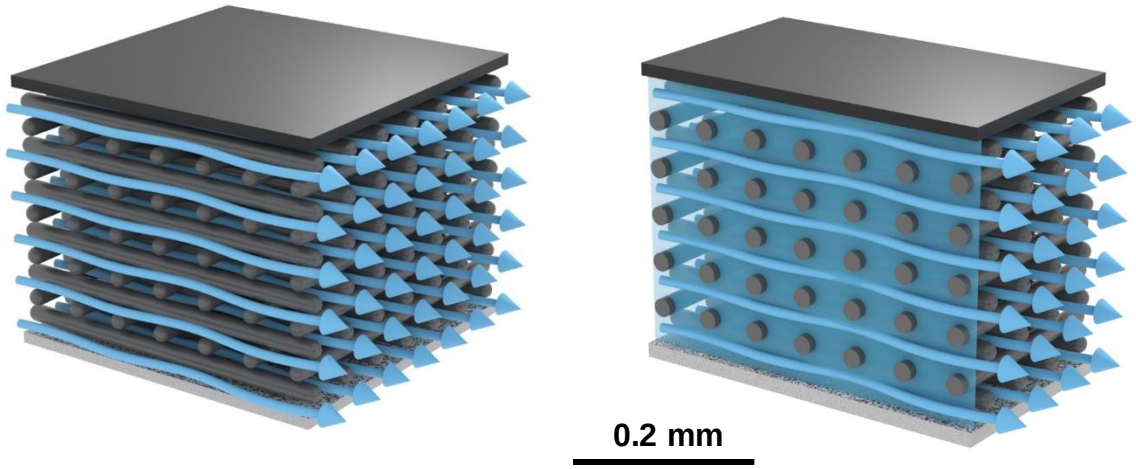


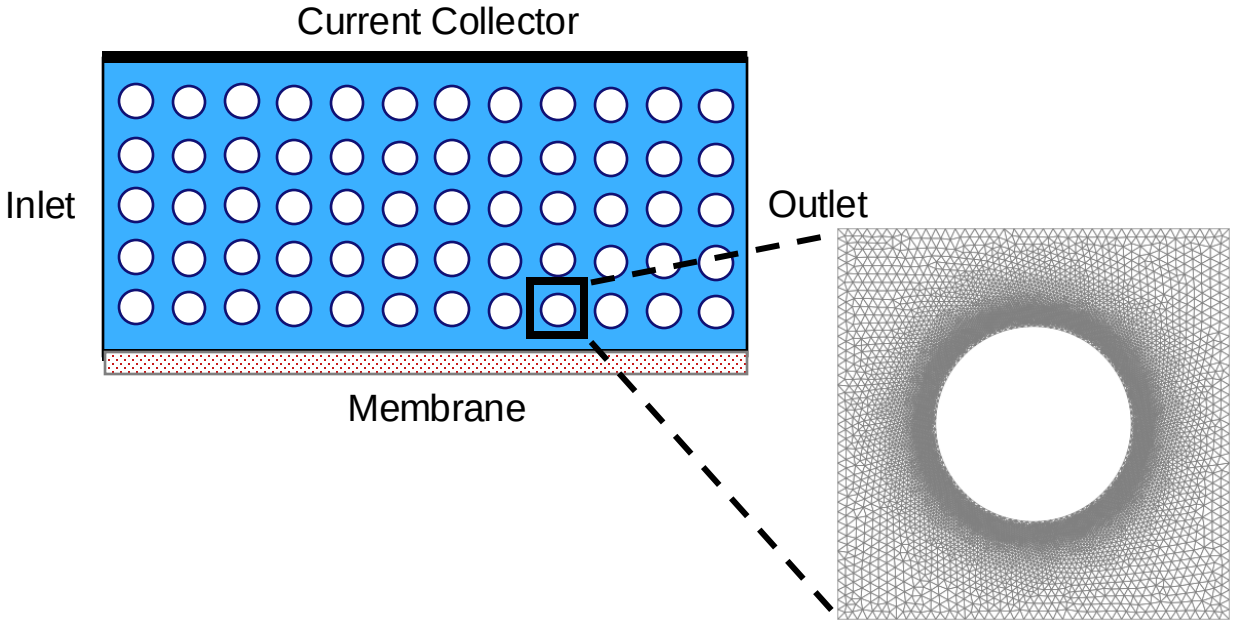
Modeling Workflow

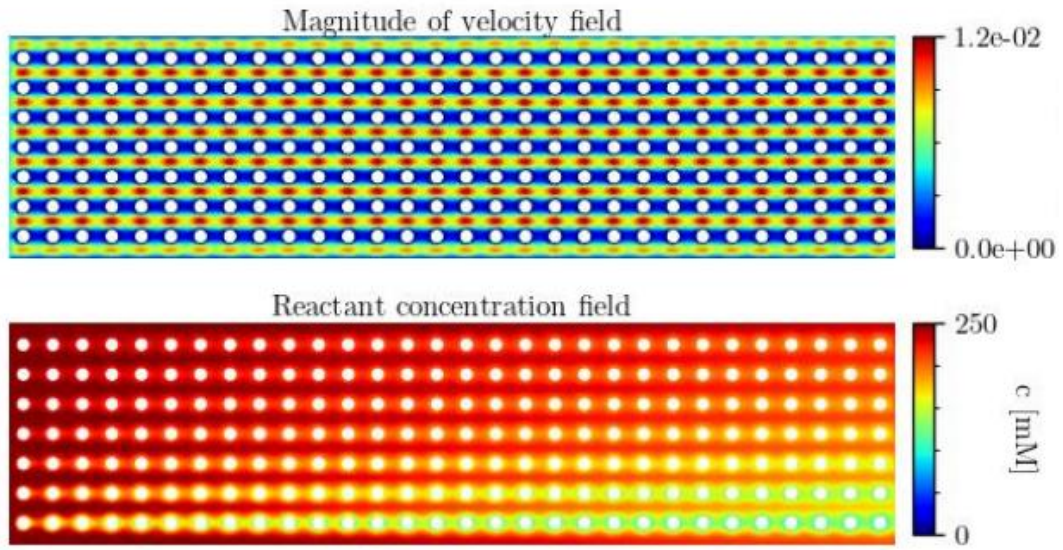


Pore-Scale Transport

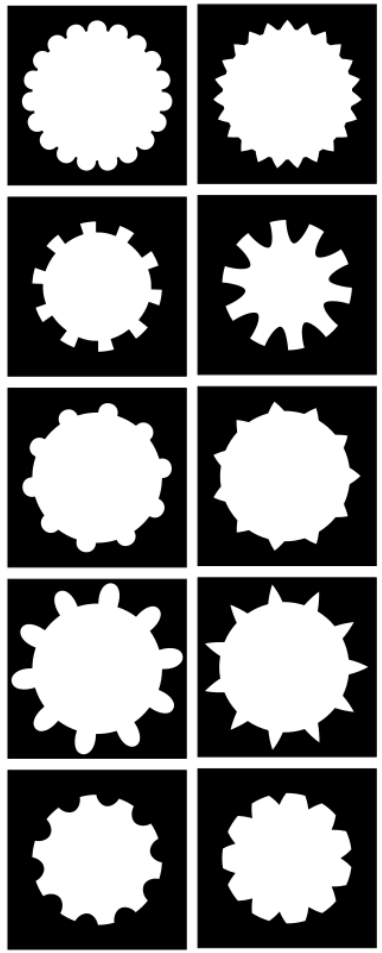


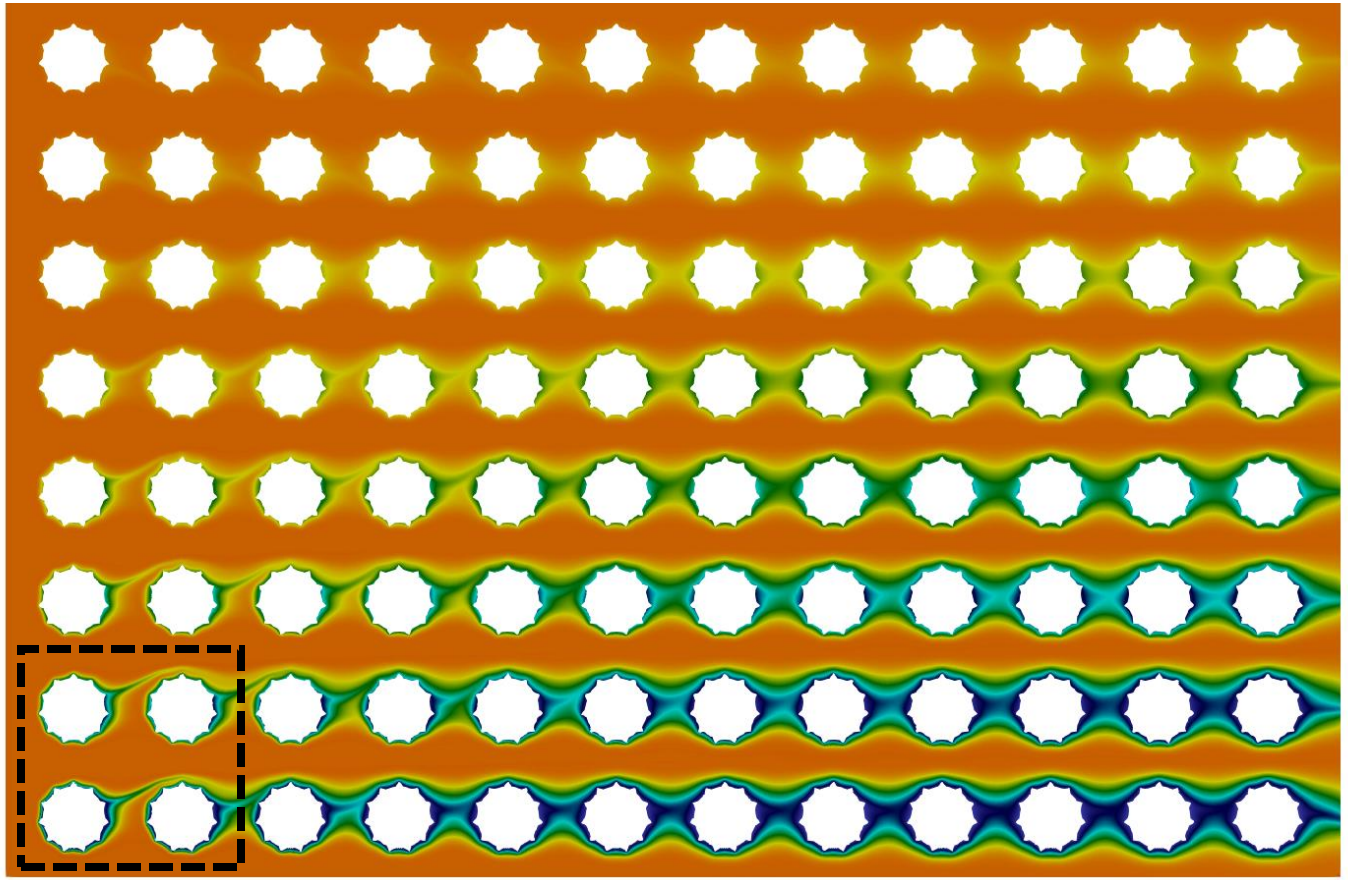


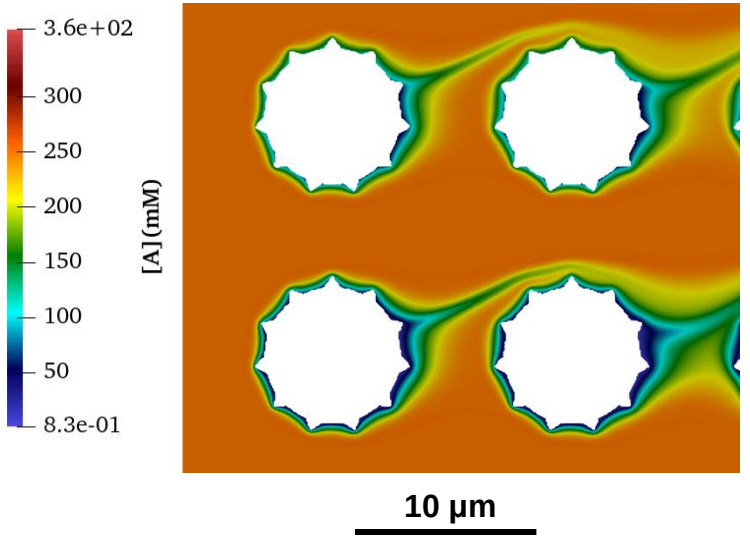




Effect of Fibers' Morphology

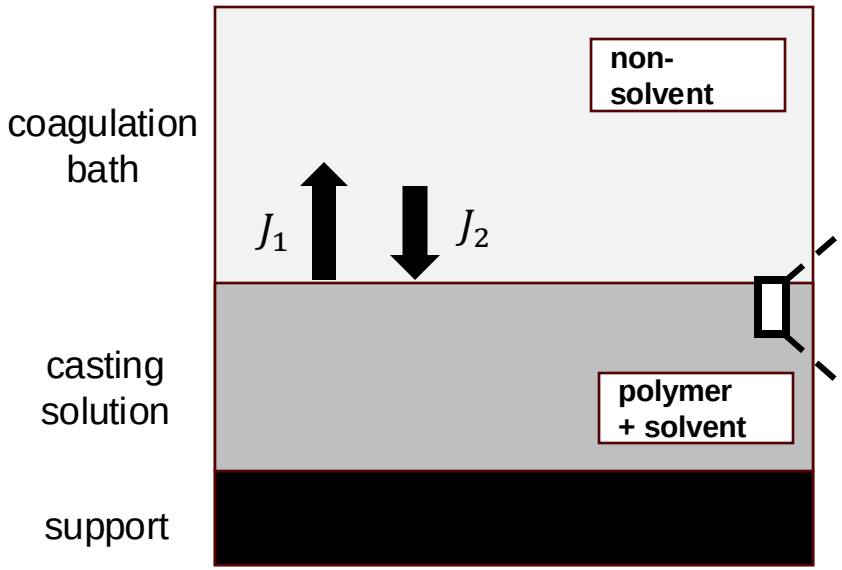


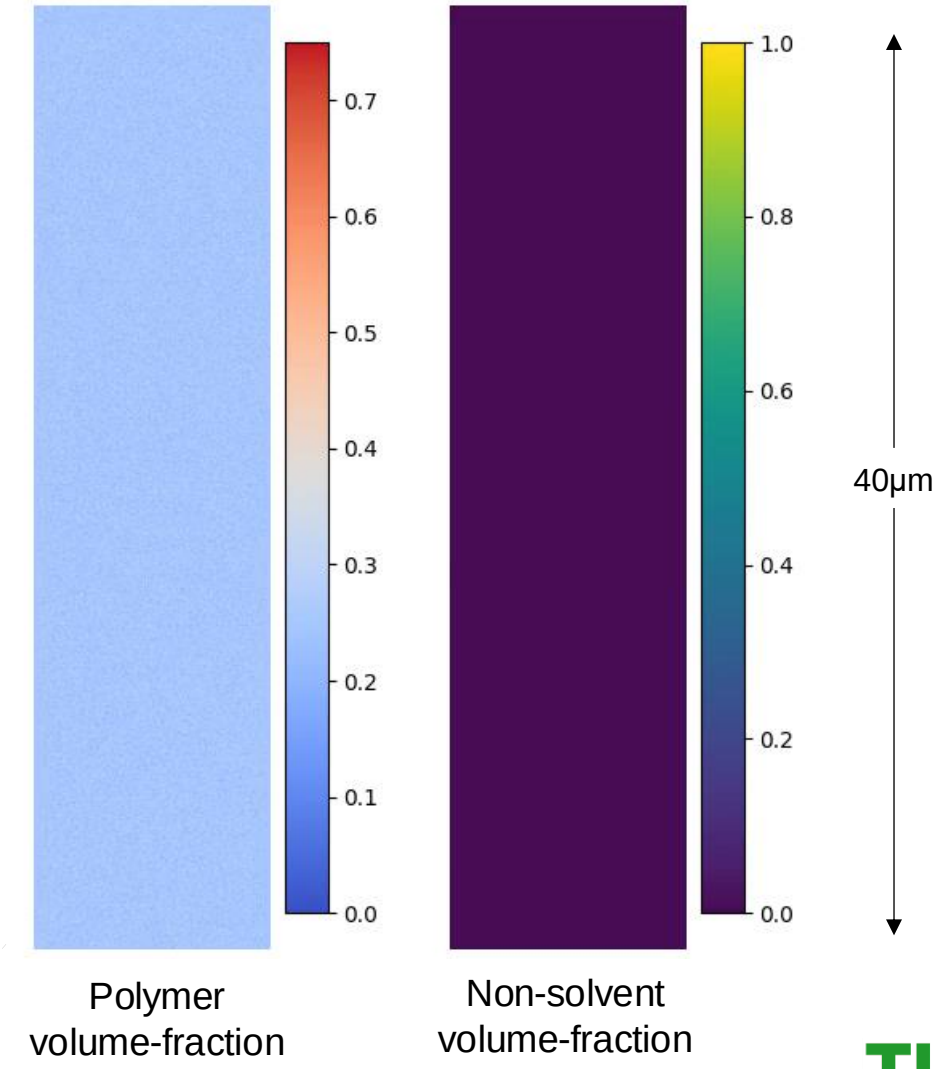




~2M elements, steady state
~9.5M DoF for Fluid Flow, ~4.5M DoF for Mass/Charge
Took ~4 minutes using 50 CPU cores

Phase Separation Model for Production Process



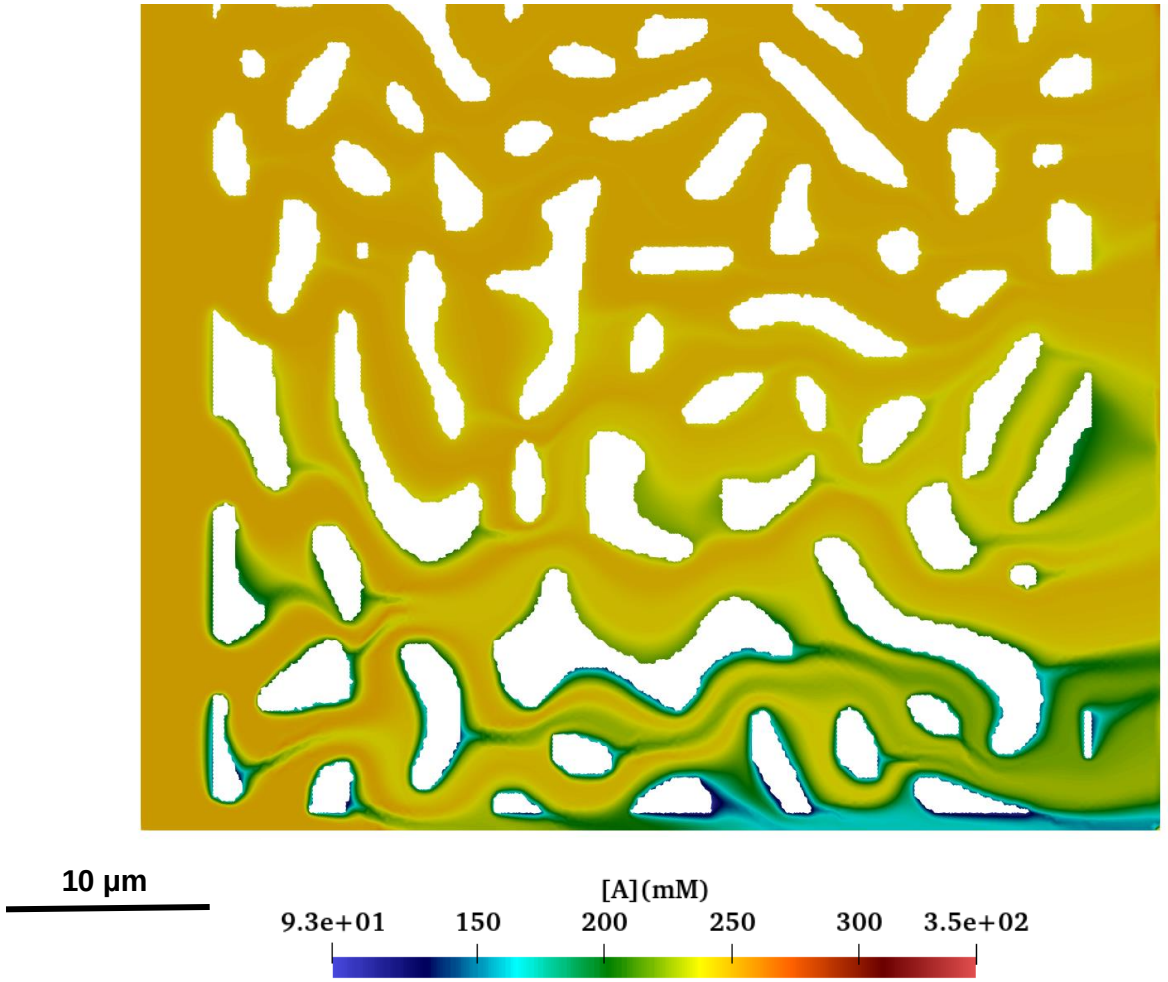


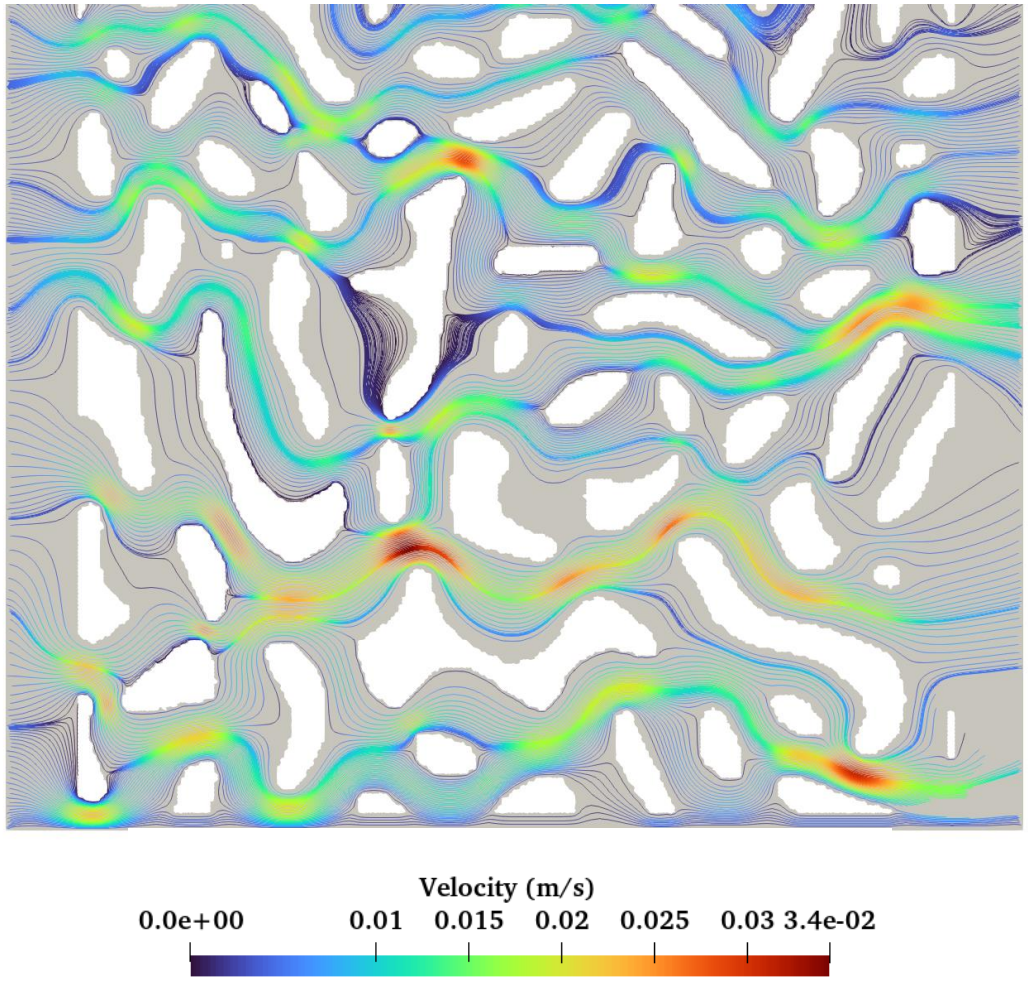
~260K elements, ~30M time steps
Took ~8 hours using NVIDIA RTX A5000 (~8K CUDA cores)
~5 hours using NVIDIA A100

3D Simulation

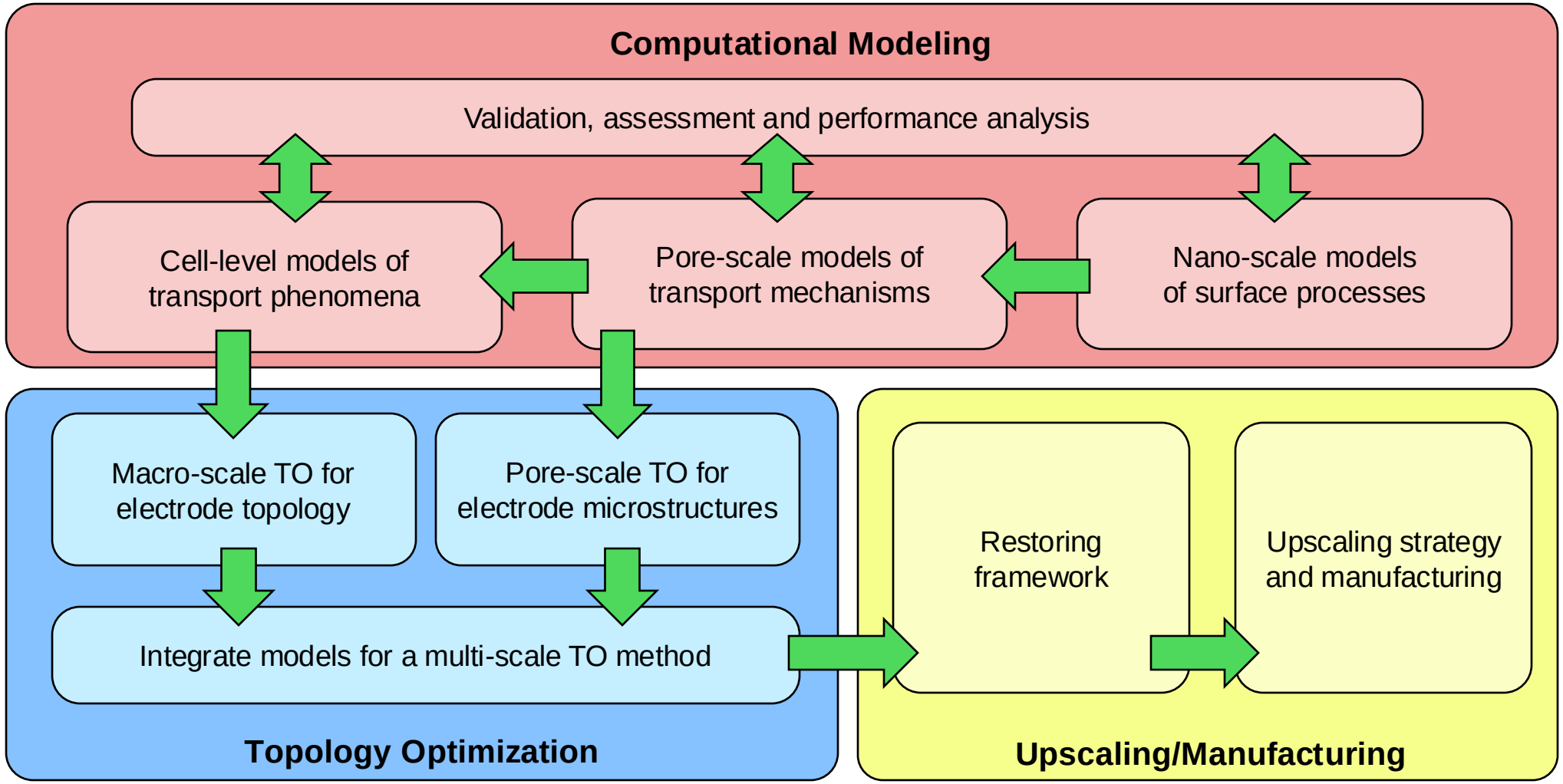
~4M elements, ~3M time steps
Took ~13 hours using NVIDIA RTX A5000 (~8K CUDA cores)

Simulating Transport in Porous Structures

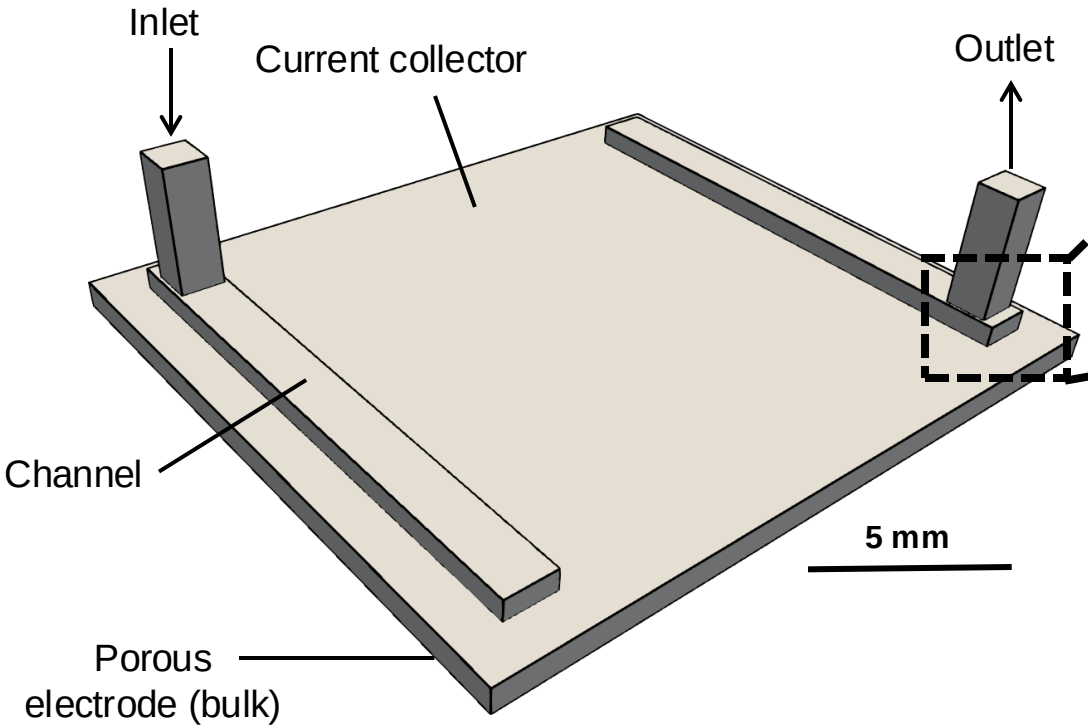


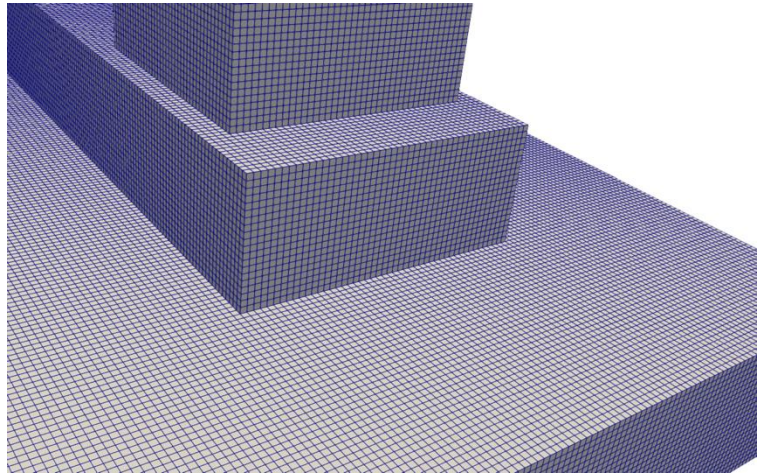


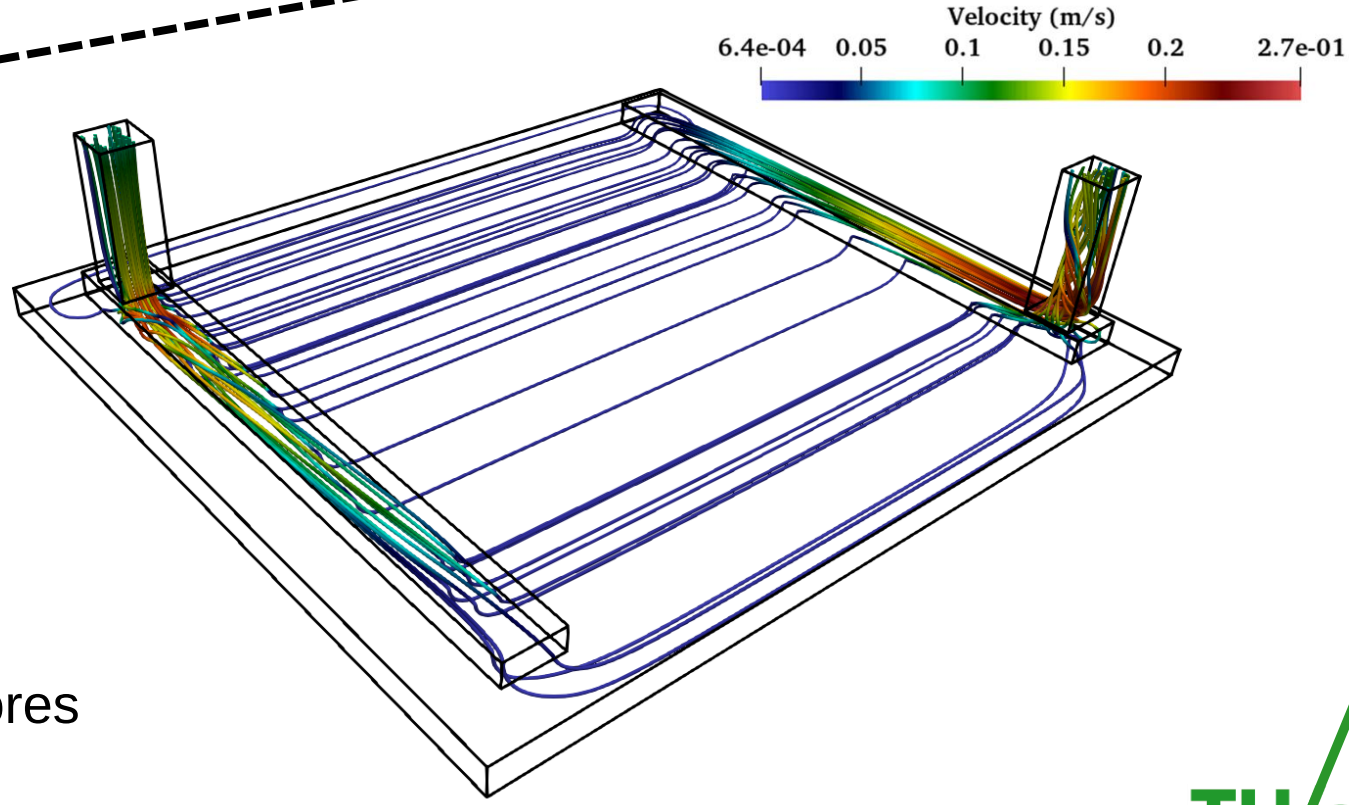
Modeling Workflow



Redox Cell-Level Transport

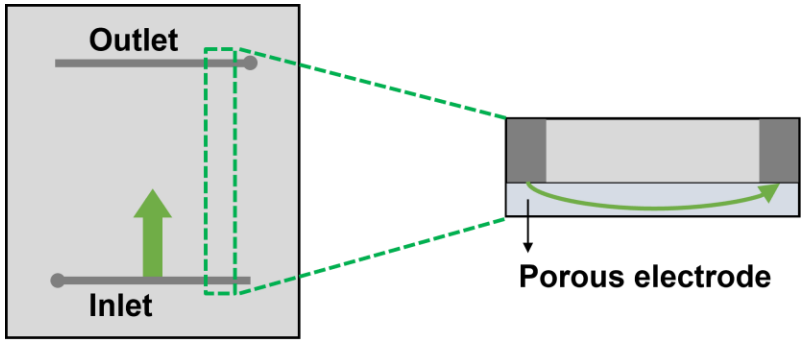


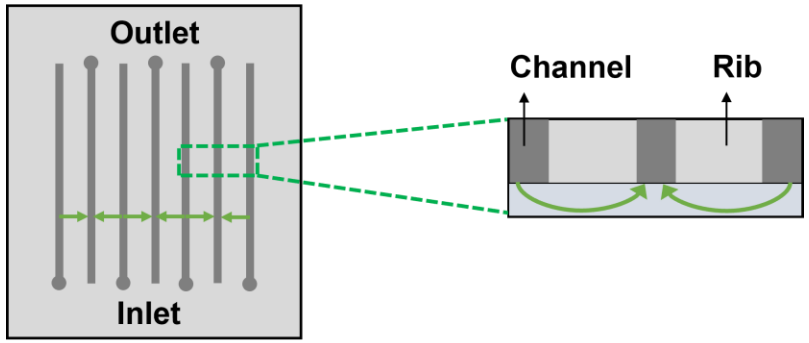


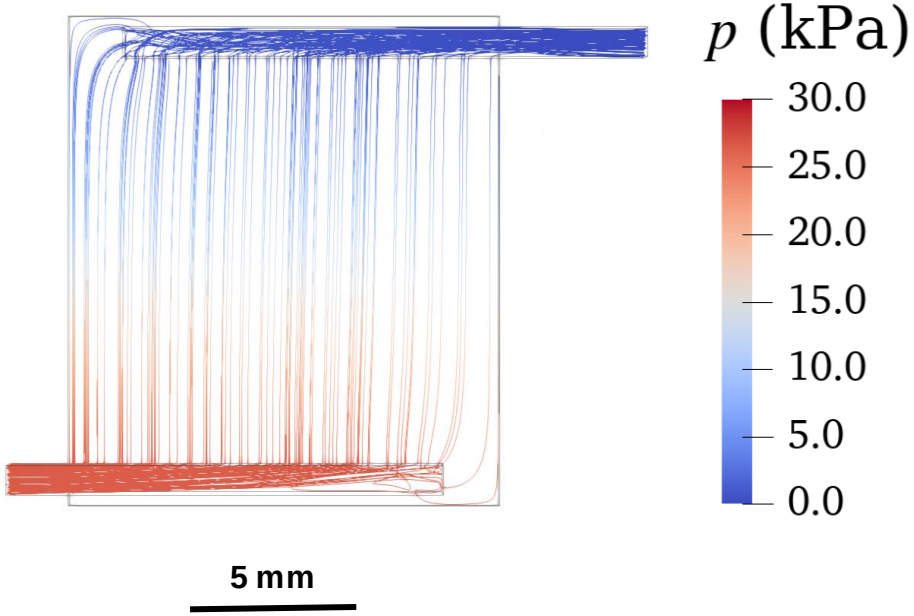


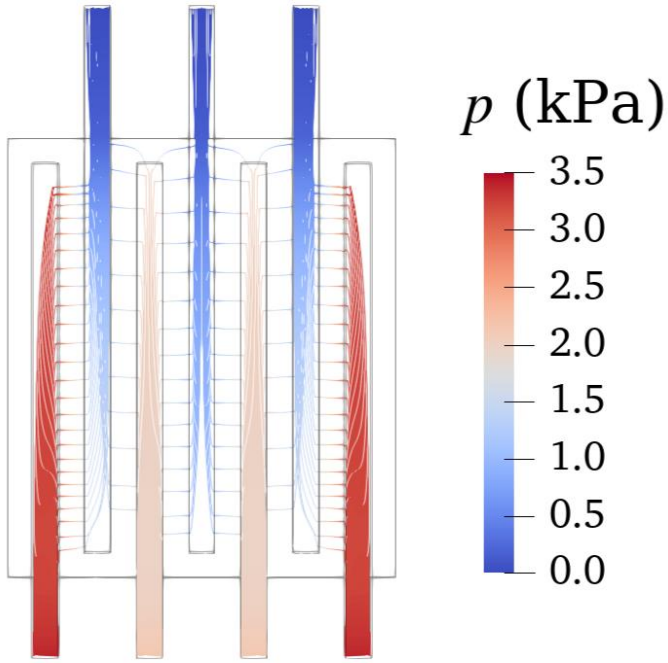
~11M elements, steady state
Took ~8 minutes using 100 CPU cores

Pressure Drop in Various Channel Setups

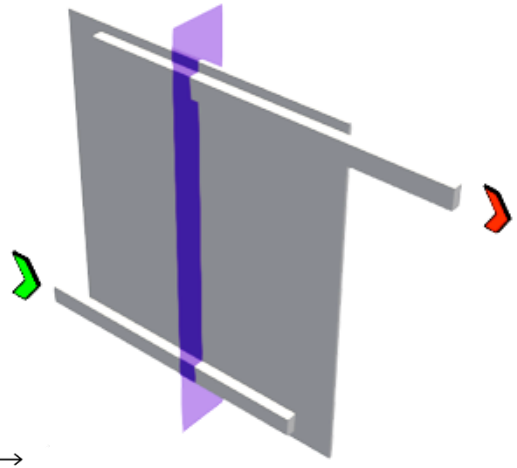


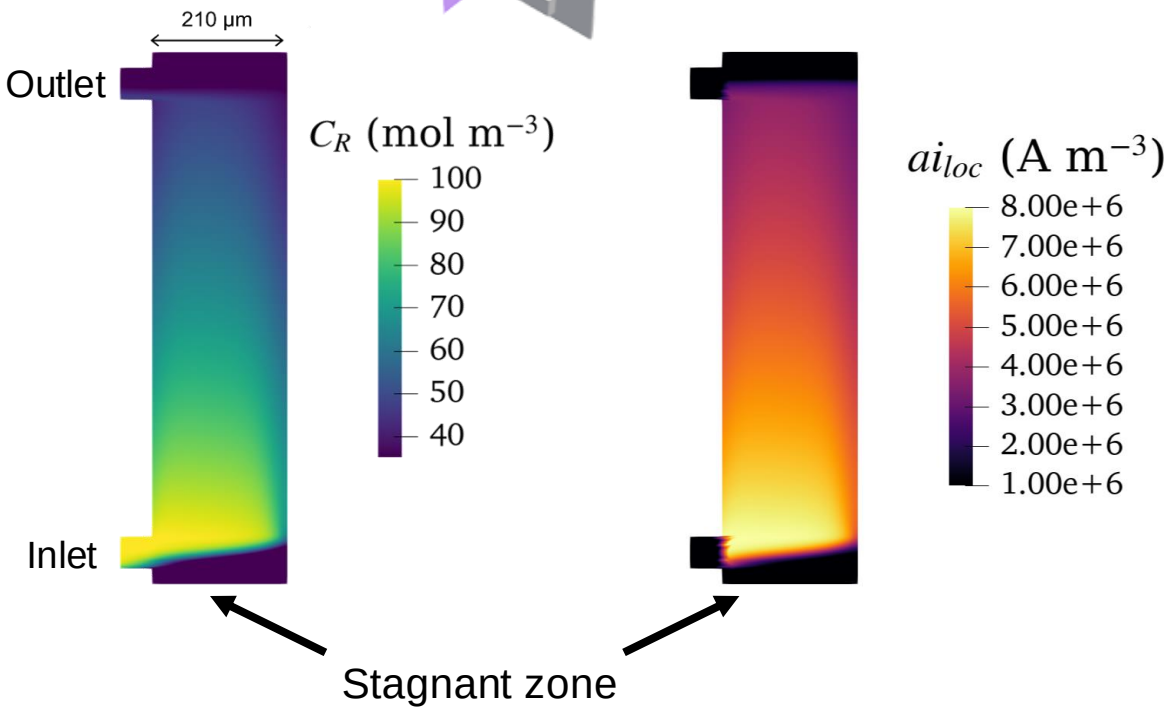


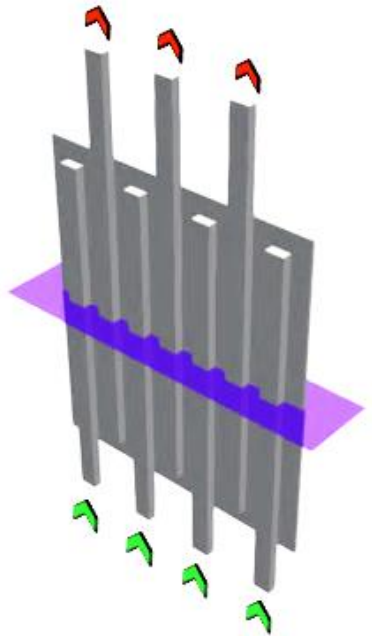




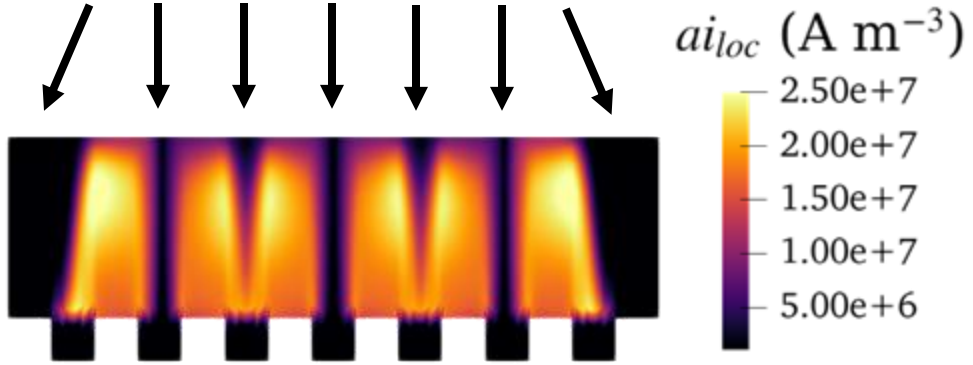
Electrode Utilization





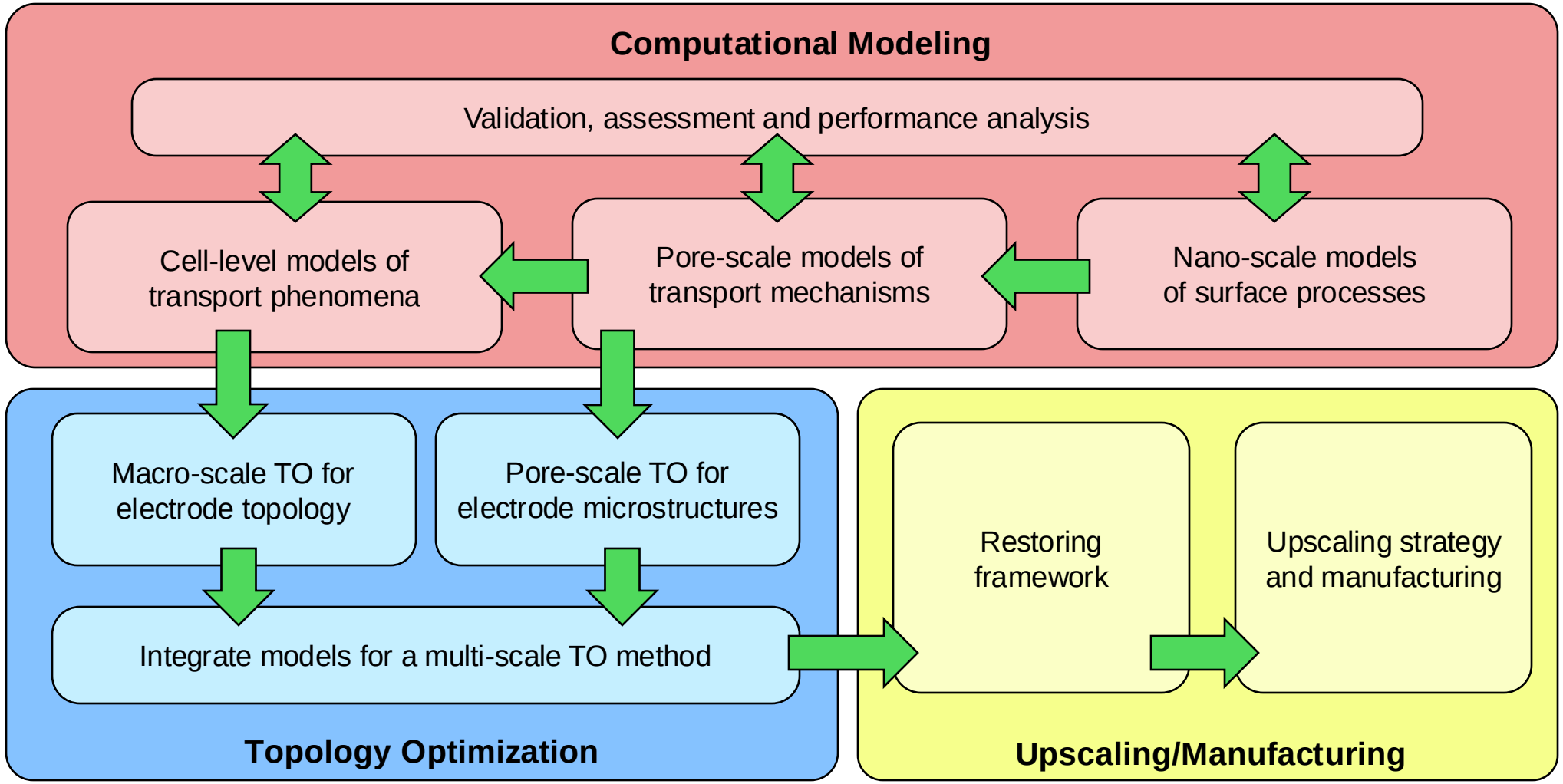


Low electrode utilization



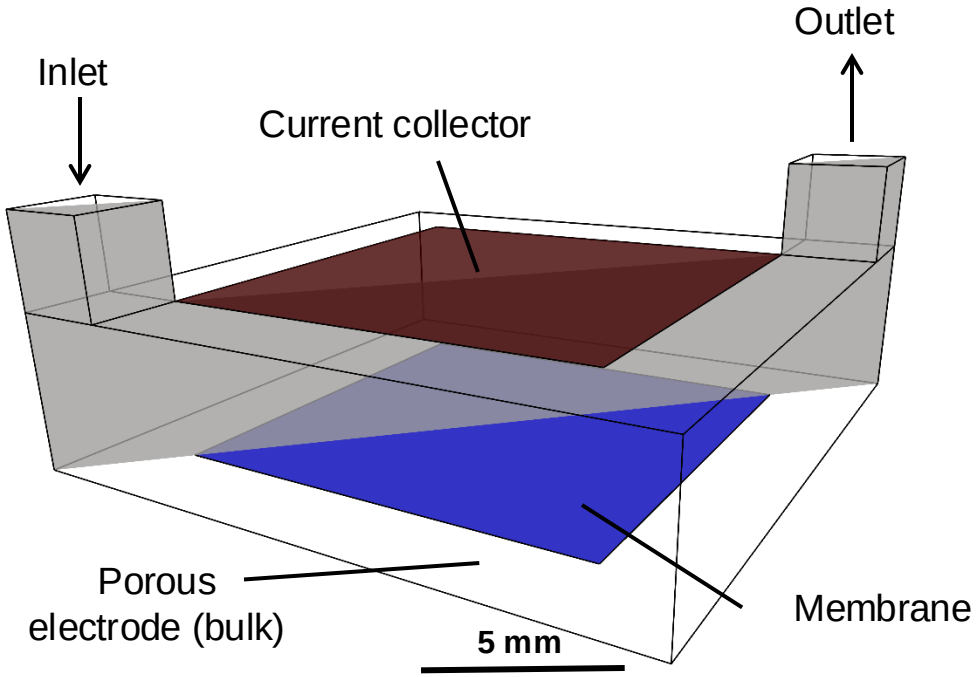
Topology Optimization of Porous Electrodes

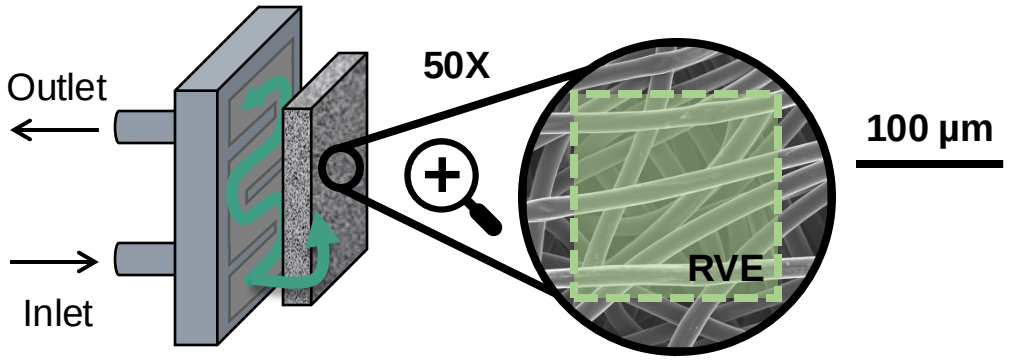
Modeling Workflow



Constructing Optimization Model

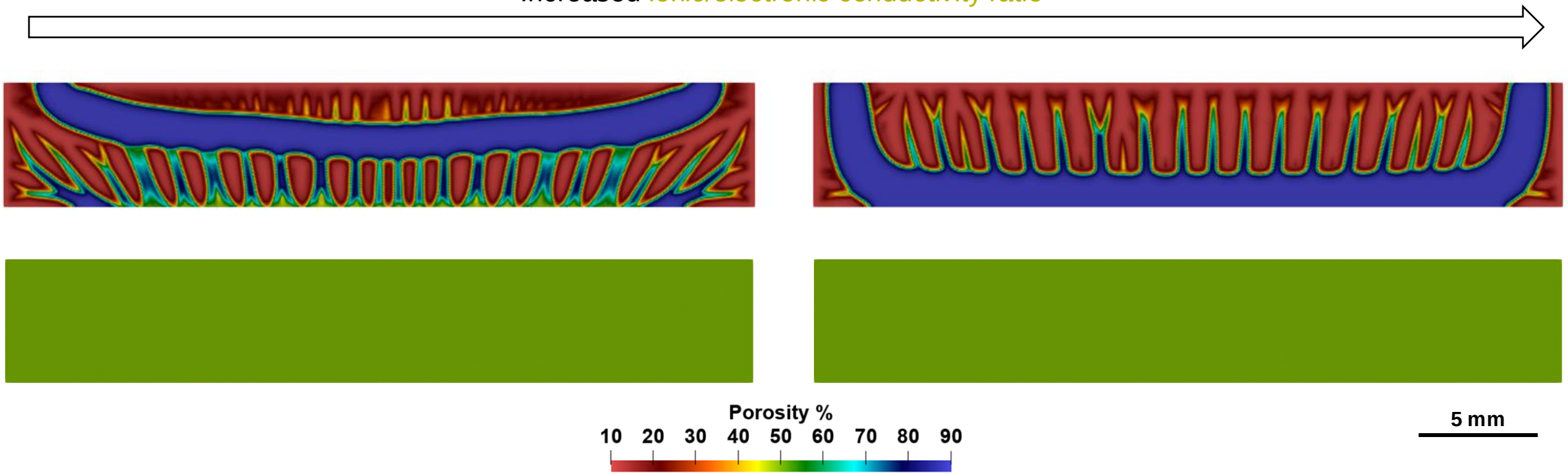
- Objective functions (targets):
  - Reducing pumping power dissipation
  - Reducing electrochemical losses





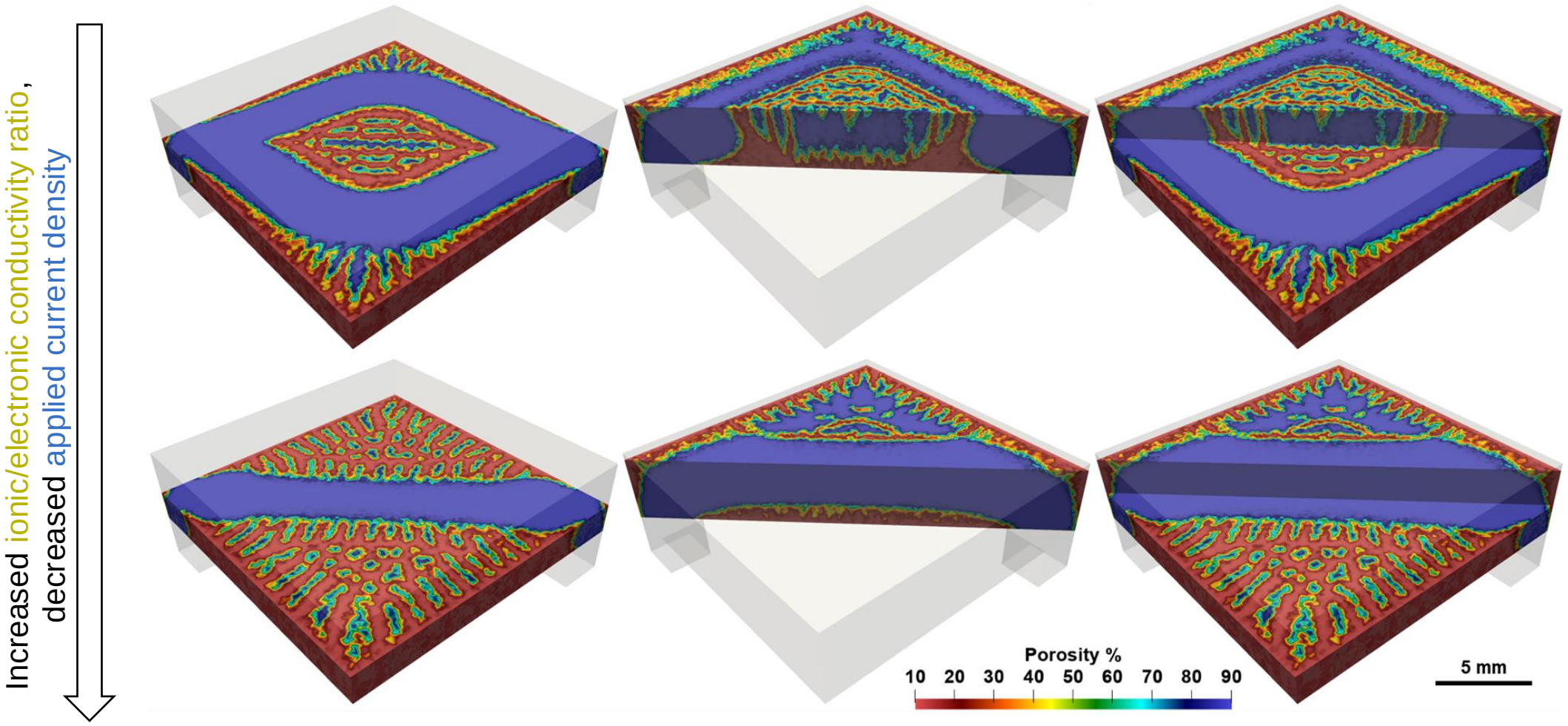
2D Simulations

Increased ionic/electronic conductivity ratio



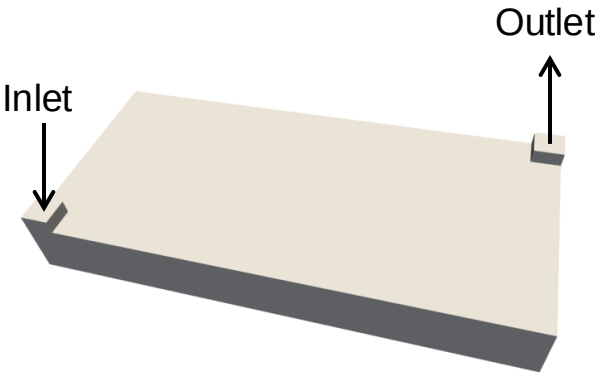
~110K elements, 150 iterations
~500K DoF for Fluid Flow, ~100K DoF for Charge
Took ~45 minutes using 16 CPU cores

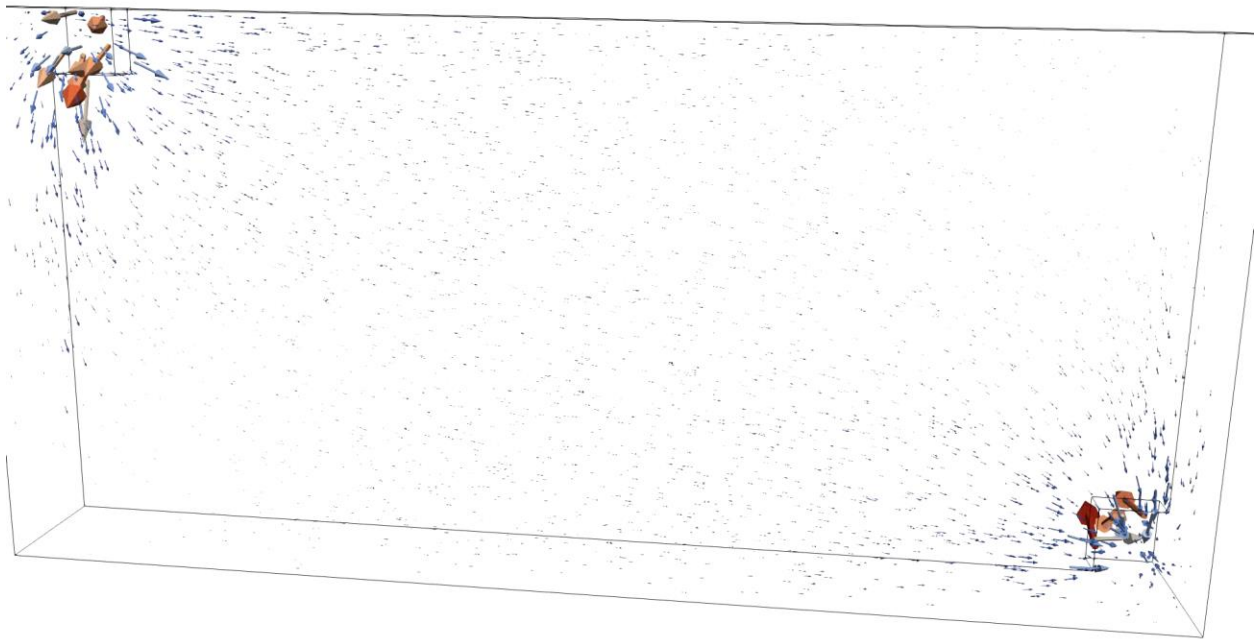
3D Simulations



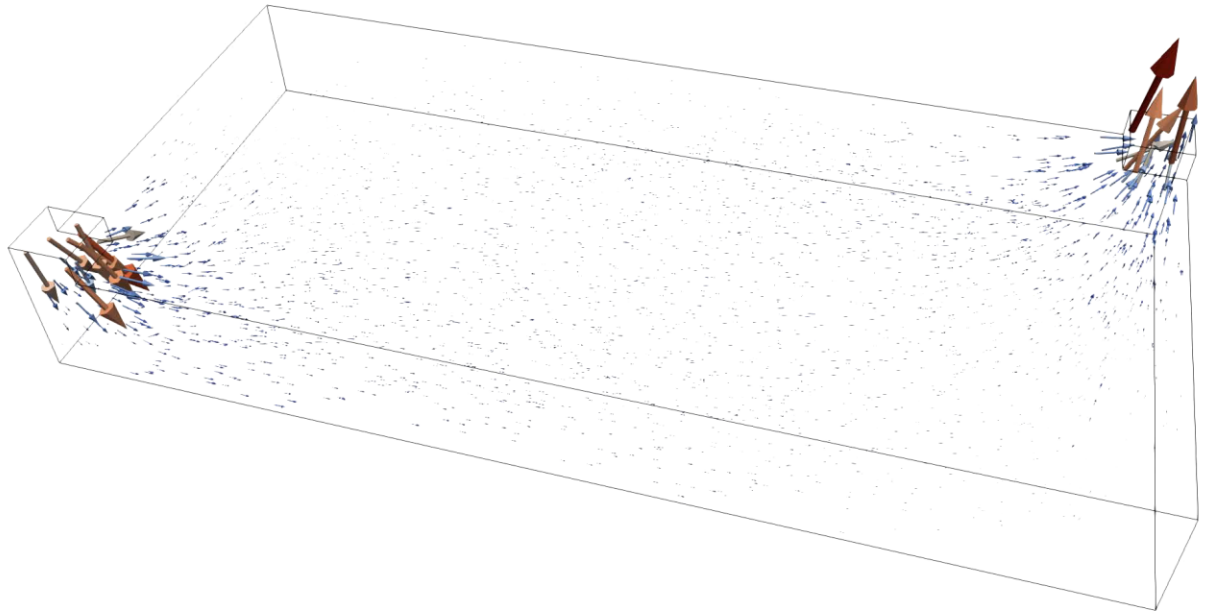
~2M elements, 150 iterations
~8M DoF for Fluid Flow, ~700K DoF for Charge
Took ~4 hours using 240 CPU cores (3 nodes)

3D Example





Bottom view

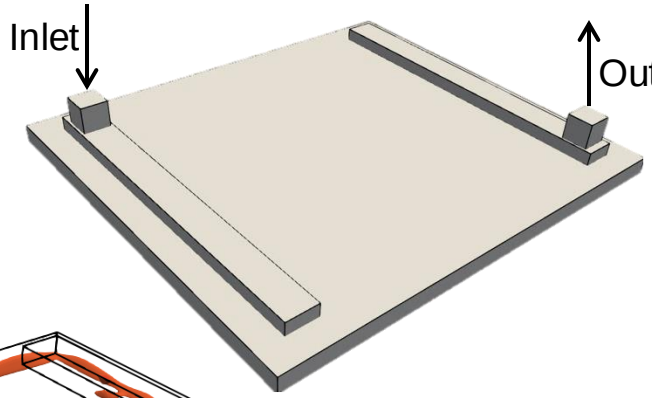


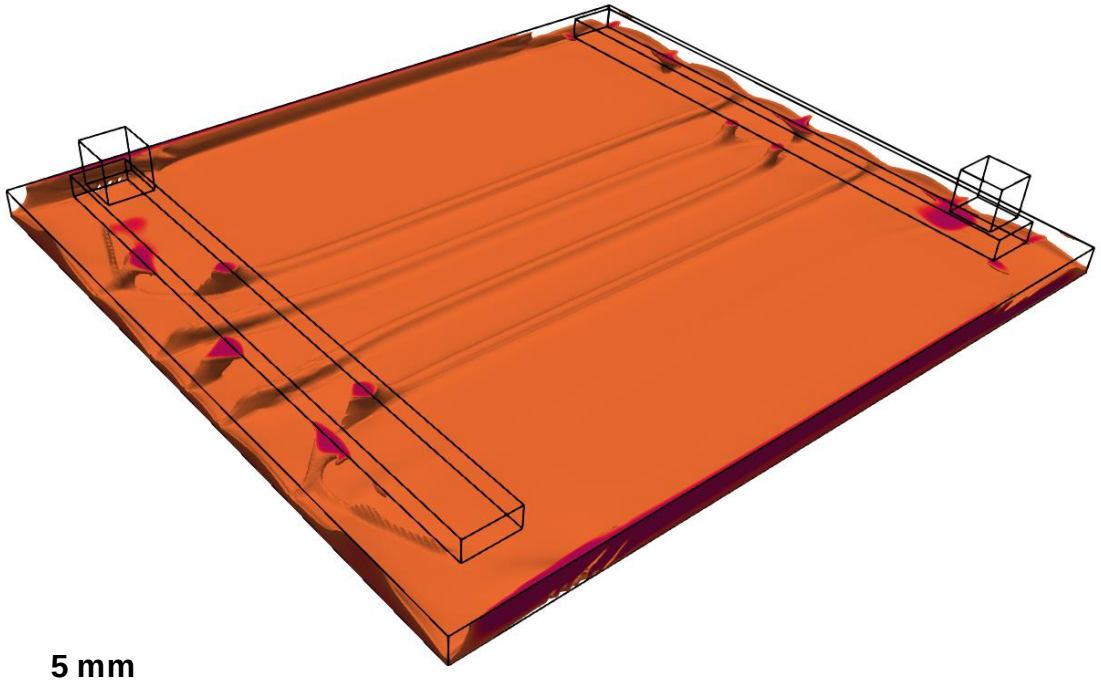
Top view

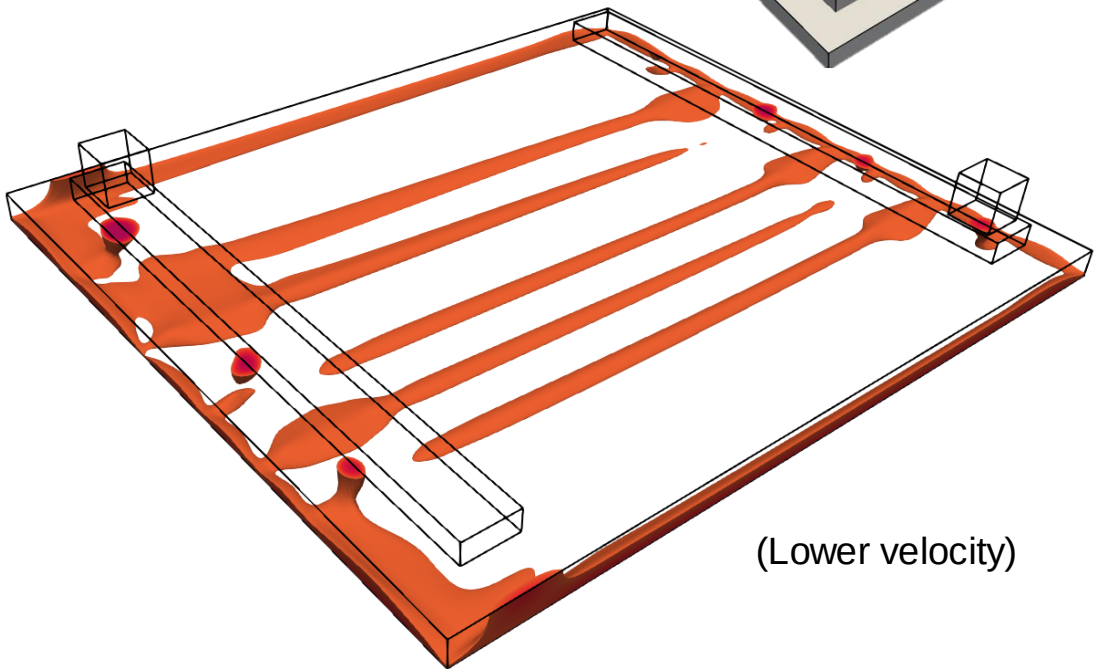
5 mm

~770K elements, 1000 iterations
Took ~4 hours using 60 CPU cores

3D Simulations with Channels

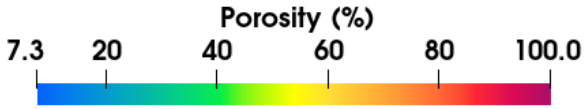






(Lower velocity)

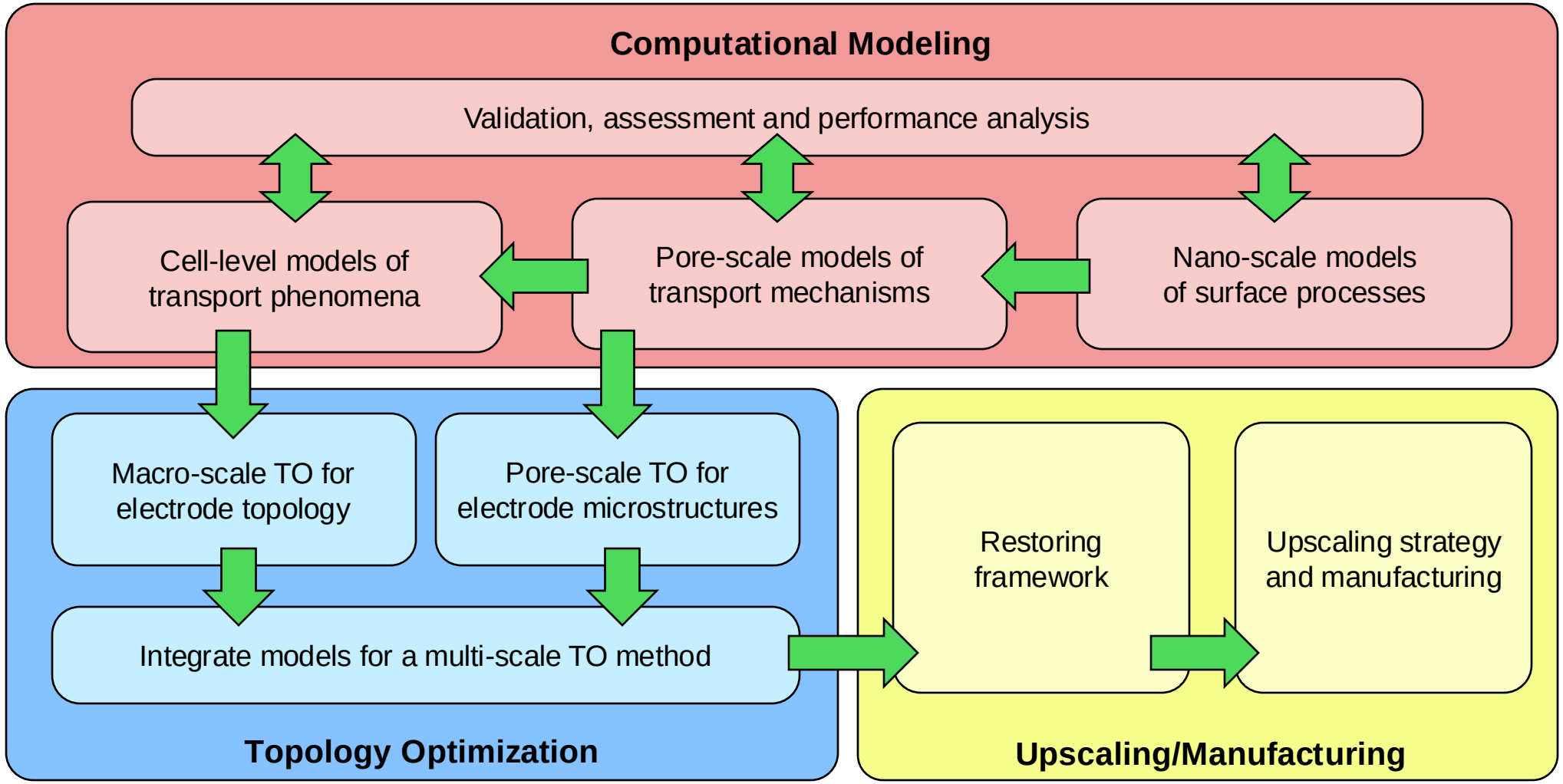
5 mm



~7M elements, 1000 iterations
Took ~21 hours using 300 CPU cores (3 nodes)

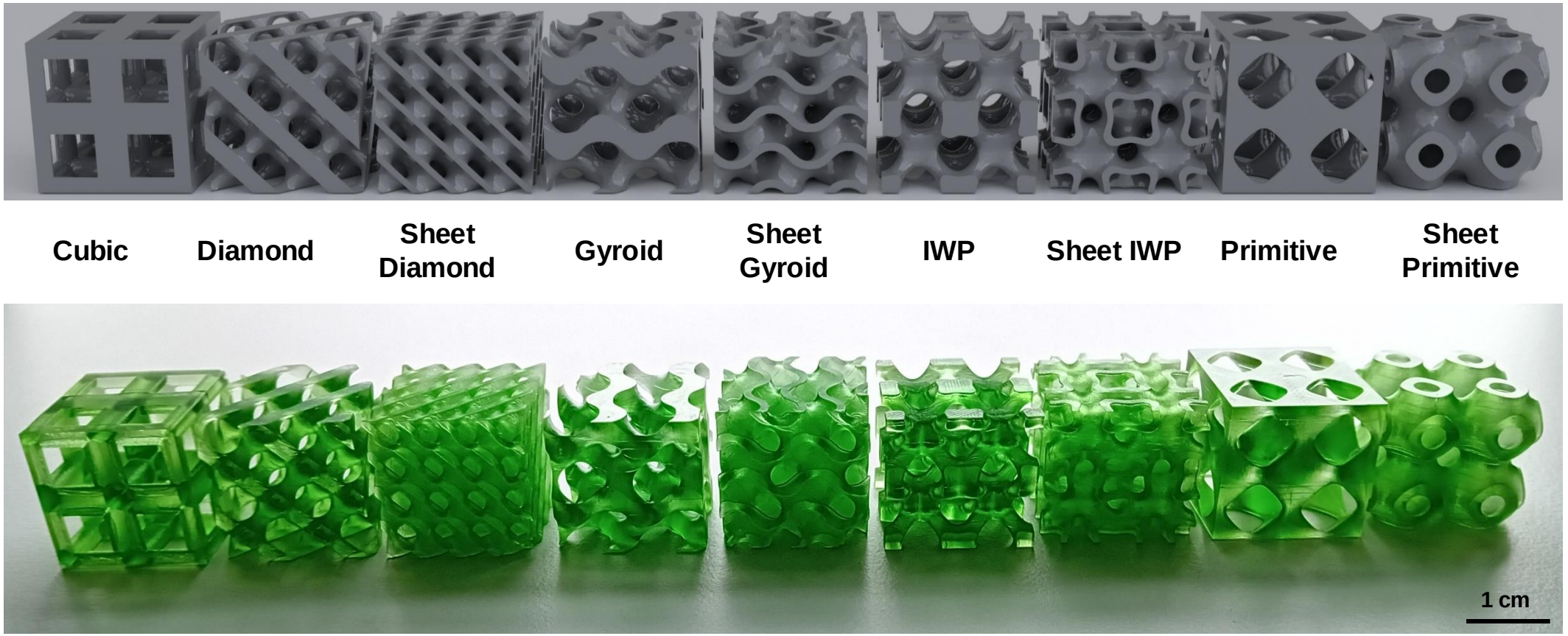
Upscaling using Periodic Surfaces

Modeling Workflow

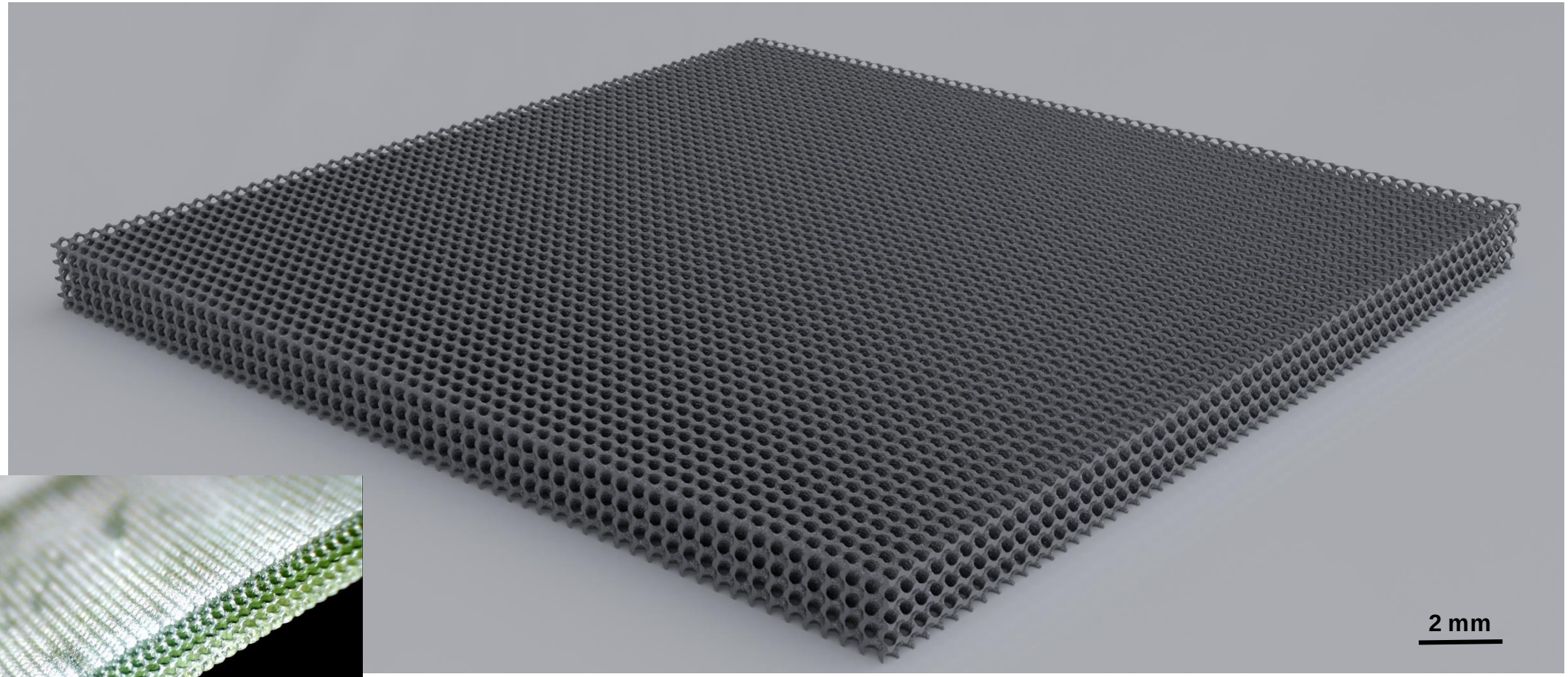


Triply Periodic Minimal Surfaces (TPMS)

- Porous infills
- Highly interconnected
- Math-friendly!
- Ability to control transport properties



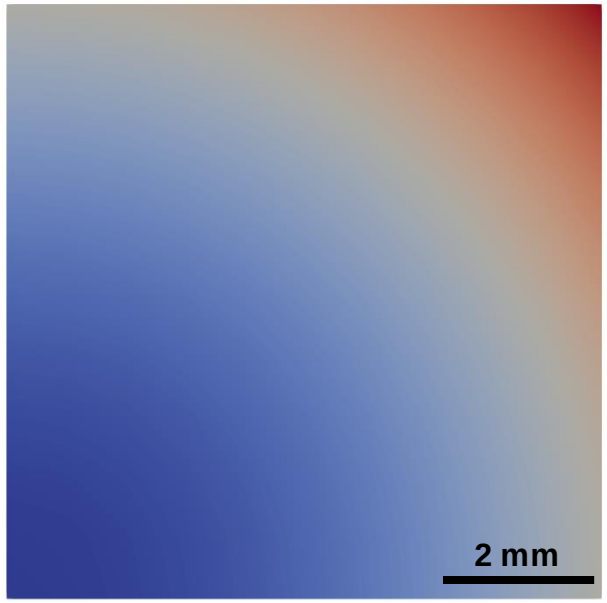
Generating Infills



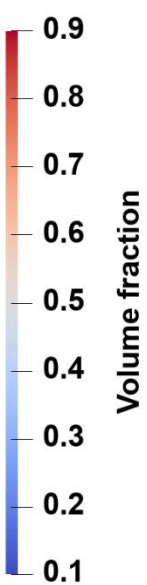
Unit cell size: 0.5 mm, Number of faces: ~ 54M
Took ~1.5 hours to generate using 64 CPU cores

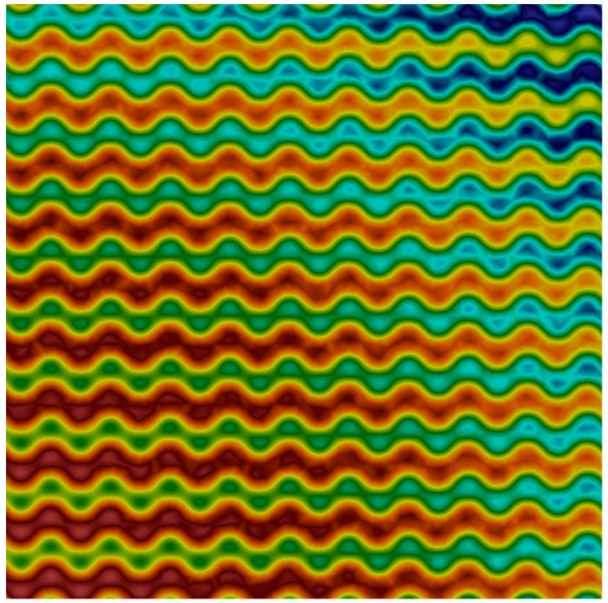
Transforming optimization results

- Converting variable porosity to TPMS infills

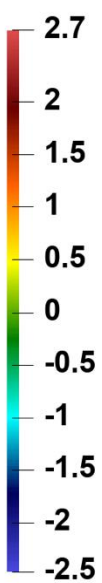


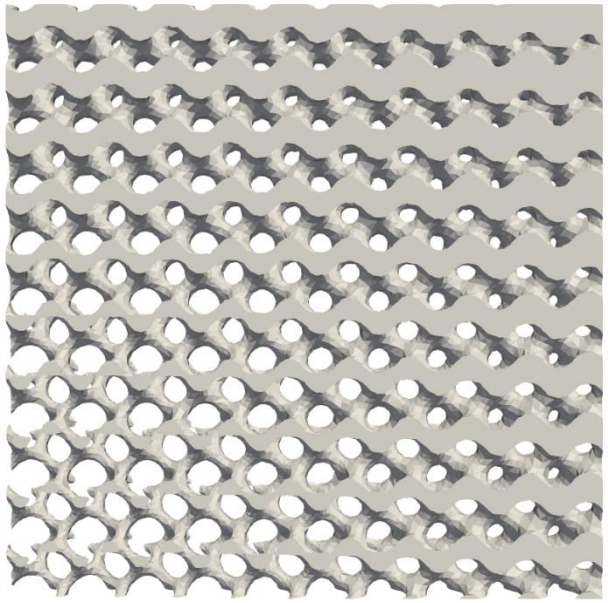
(Volume fraction)





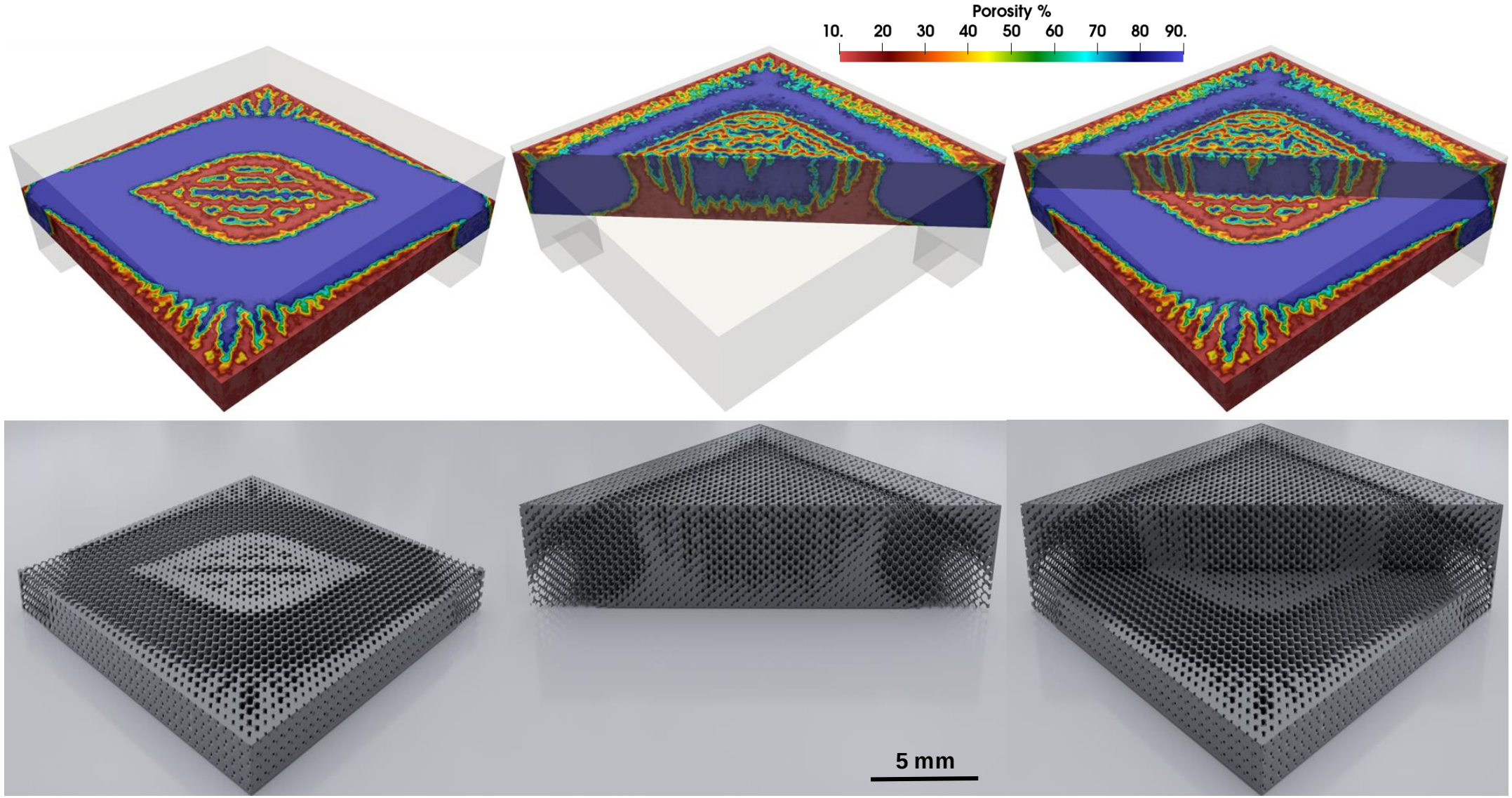
(Distance function)



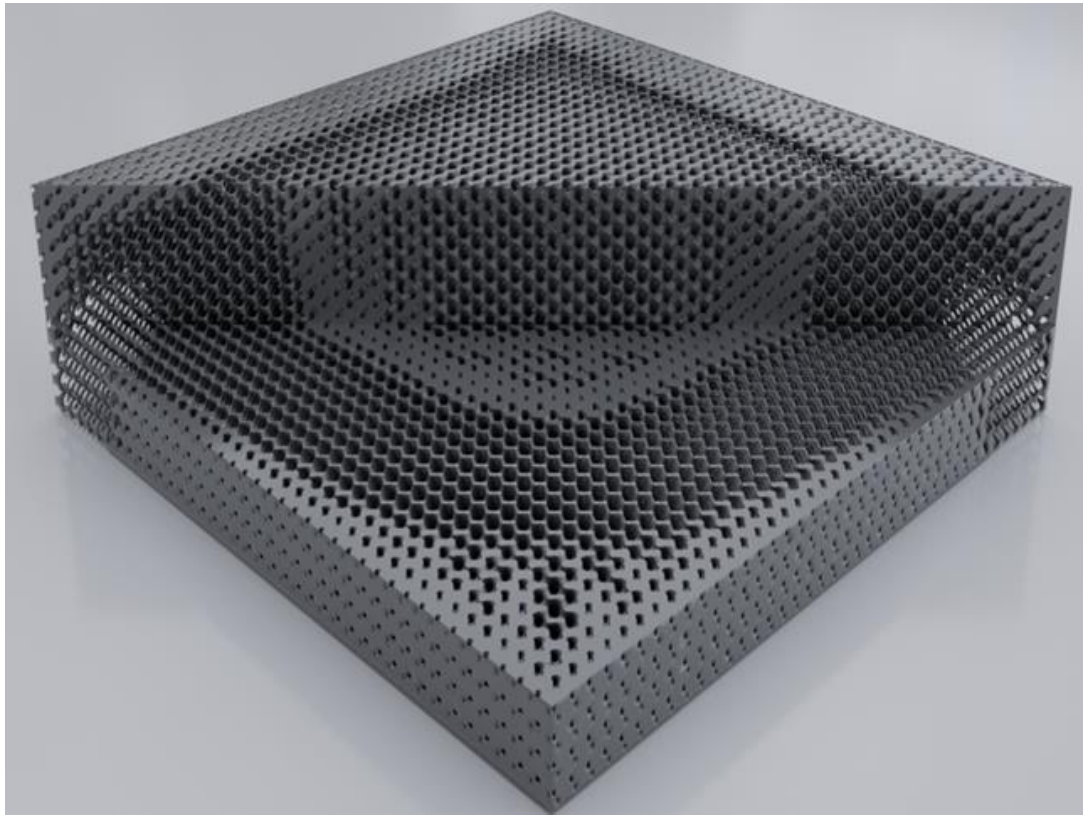


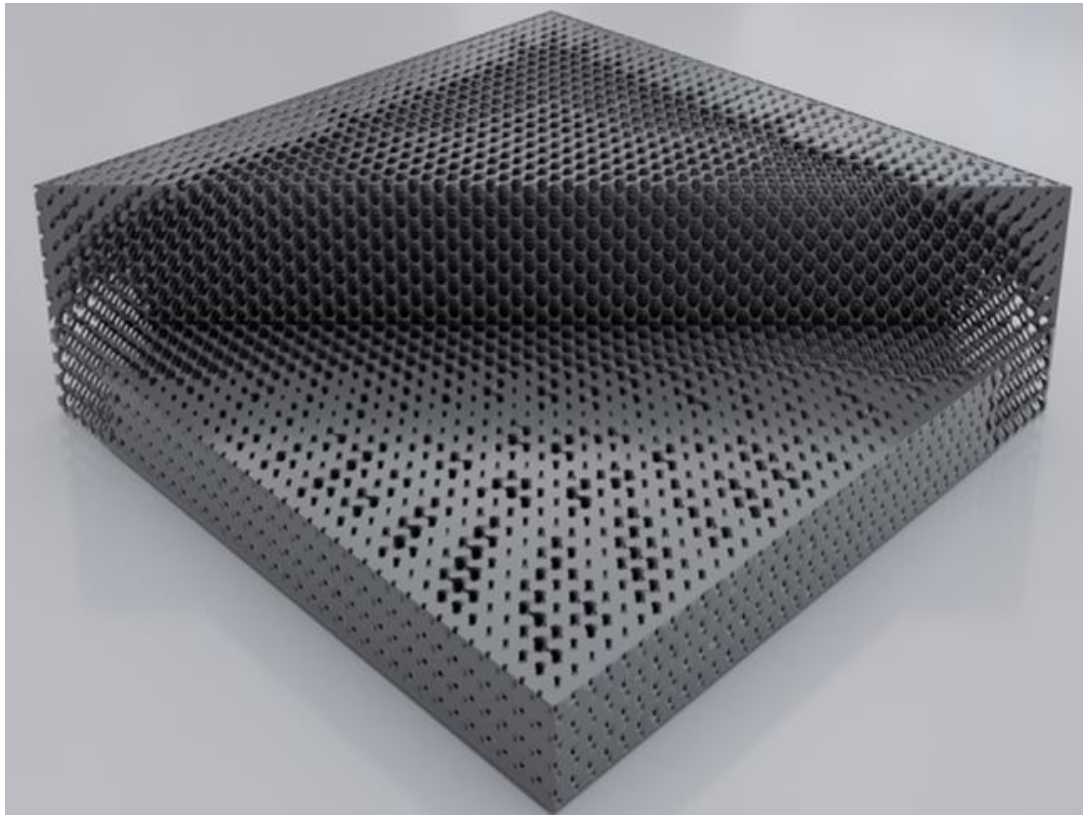
(TPMS infill)

Conversion Example



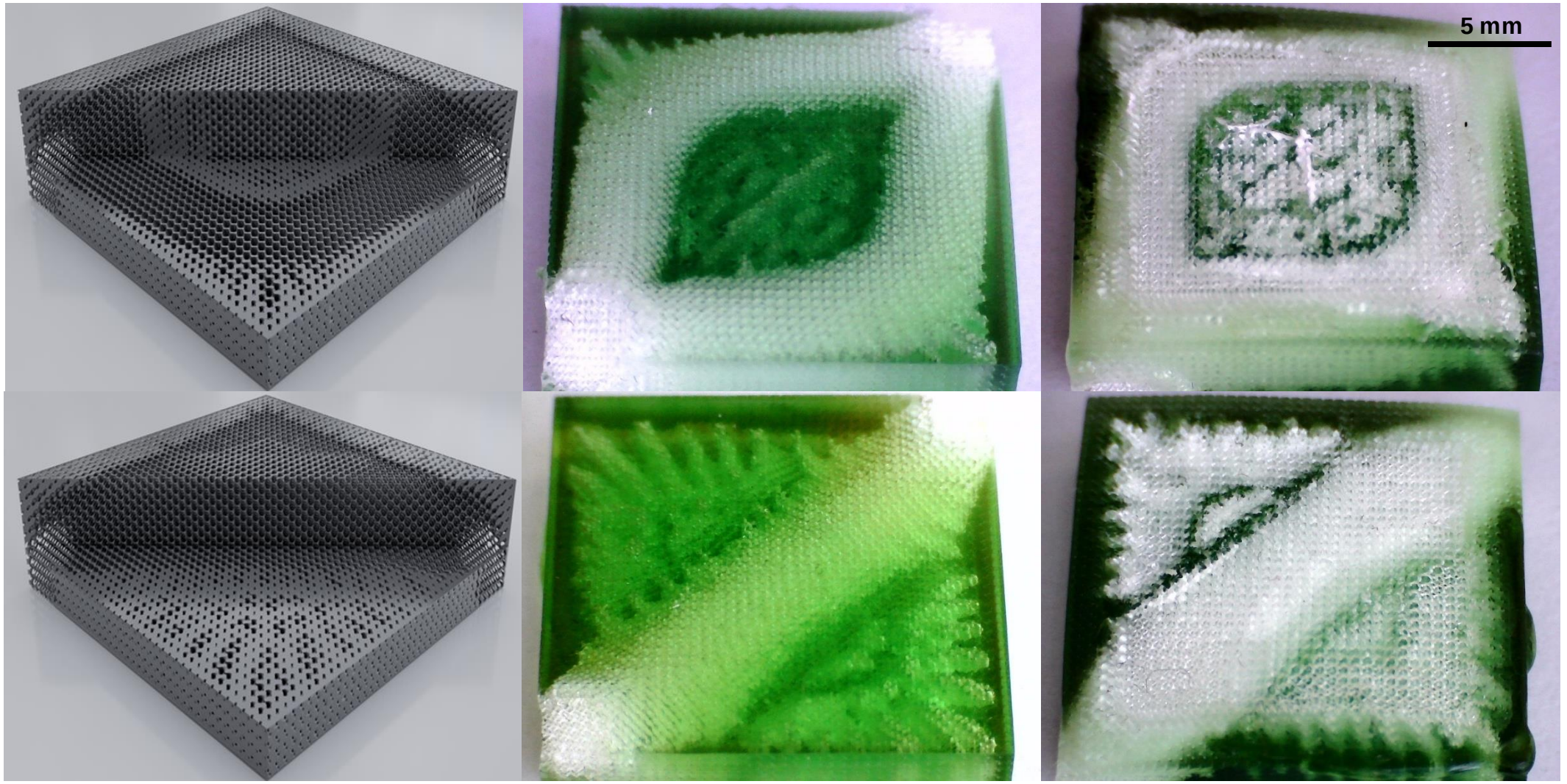
Conversion Performance



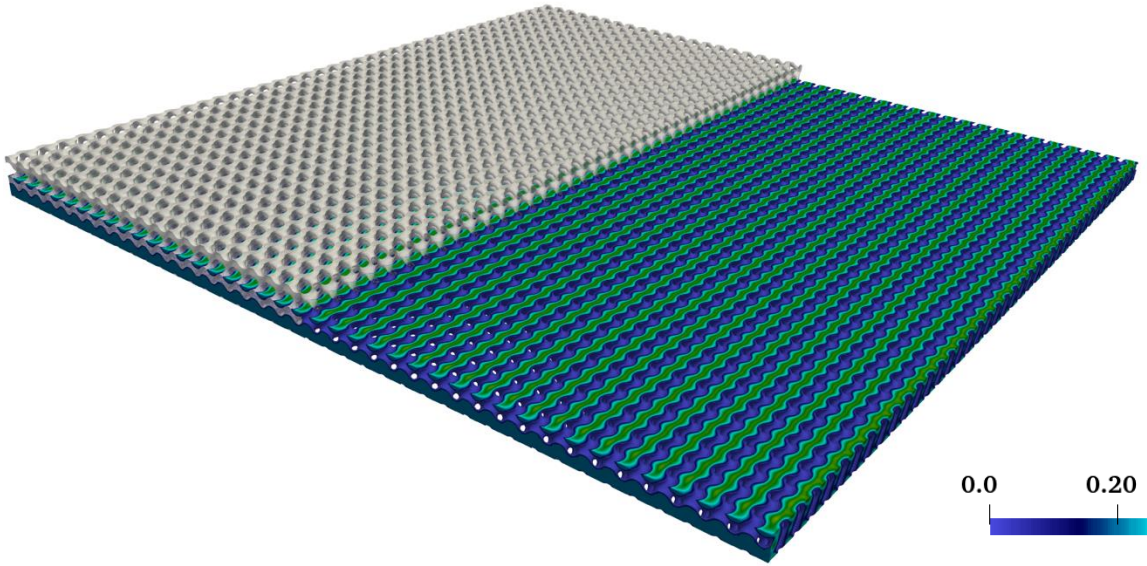


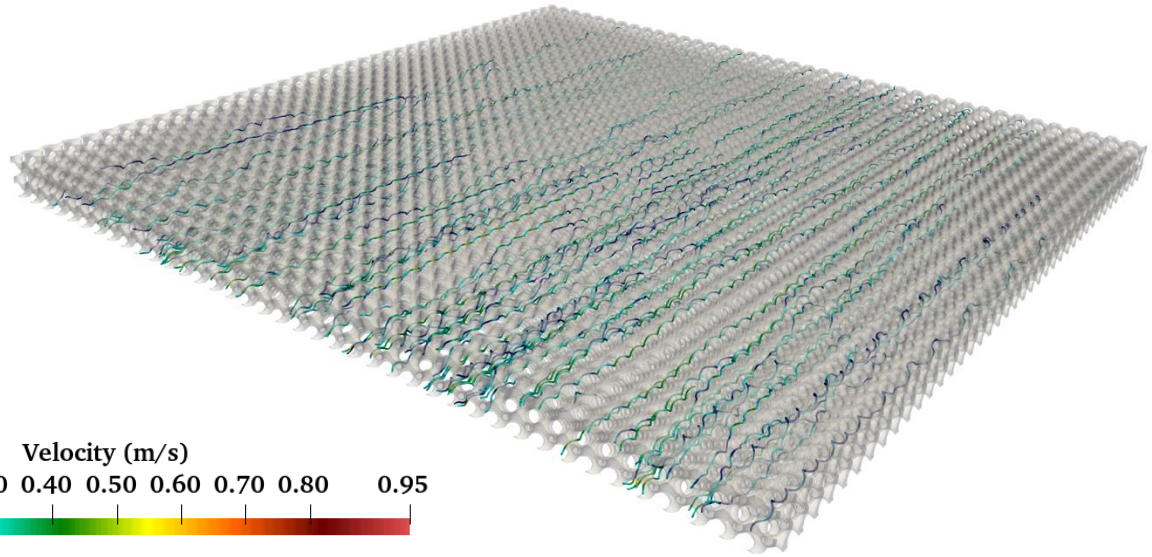
Unit cell size: 0.5 mm, Number of faces: ~ 25M
Took ~2 hours to generate using 64 CPU cores

3D Printed Electrodes

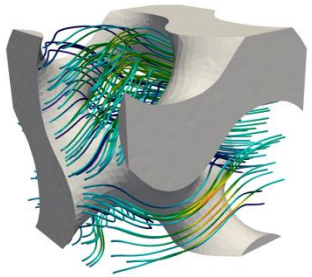


Simulating Transport Through Infills

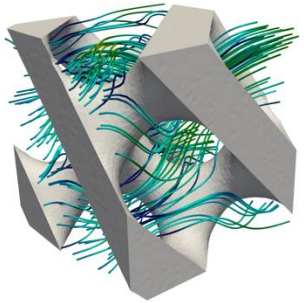




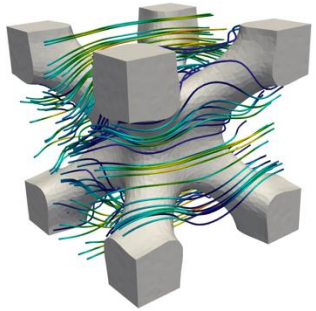
Gyroid



Diamond

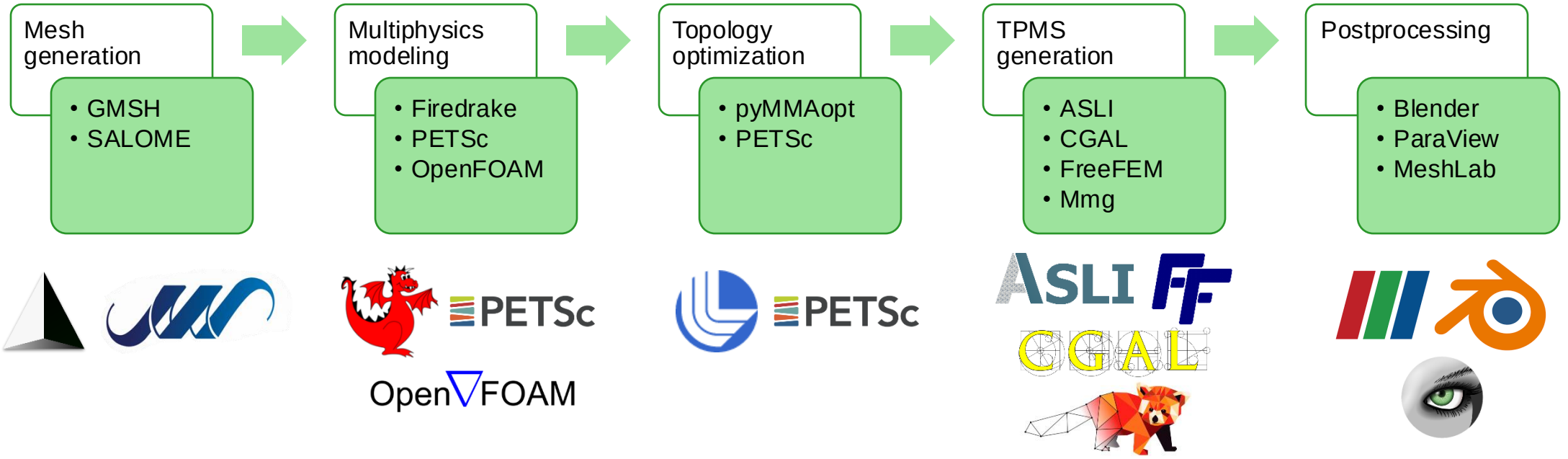


IWP



~77M DoF for Fluid Flow, steady state
Took ~50 minutes using 500 CPU cores (5 nodes)

Employed Tools are all Open-Source!



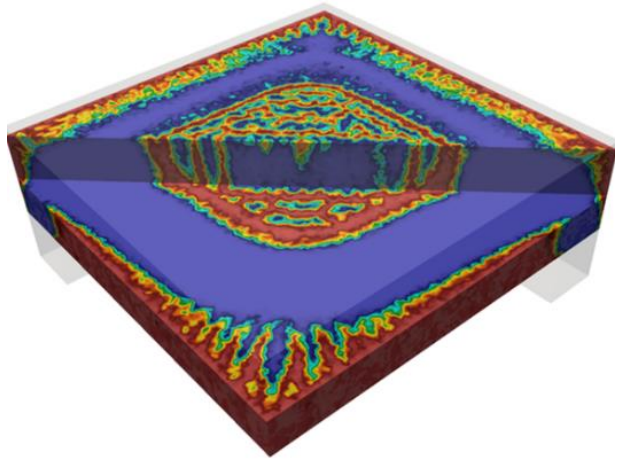
https://github.com/mbarzegary/RedOx-TO

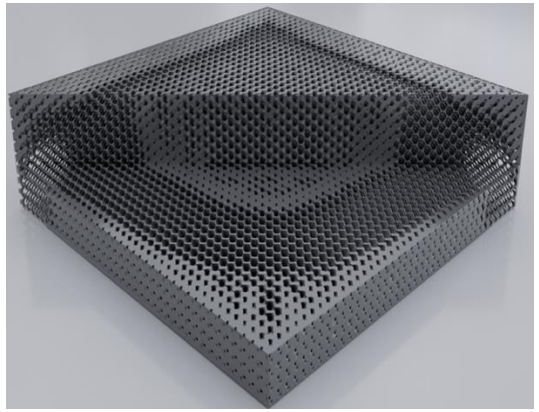
https://github.com/mbarzegary/RfbFoam

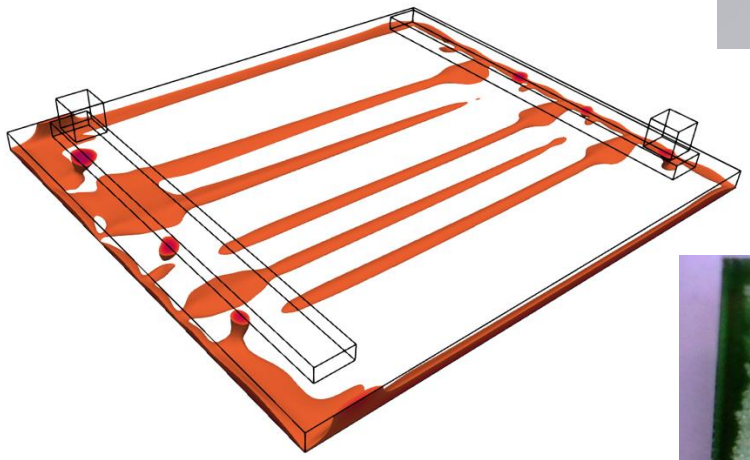
(More to be shared soon!)

Conclusion

- Numerical models for correlating local configuration/structure to overall redox cell performance
- Scalable topology optimization for engineering porous electrodes
- Manufacturability by transforming results to TPMS infills







Thank You for Your Attention!

mbarzegary.github.io

fornercuencaresearch.com