Pore-Scale Analysis of Electrochemical Devices (with OpenPNM)

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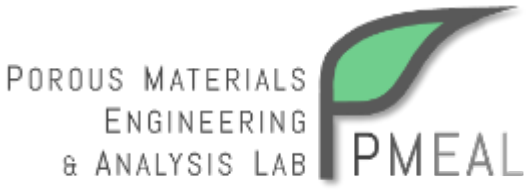
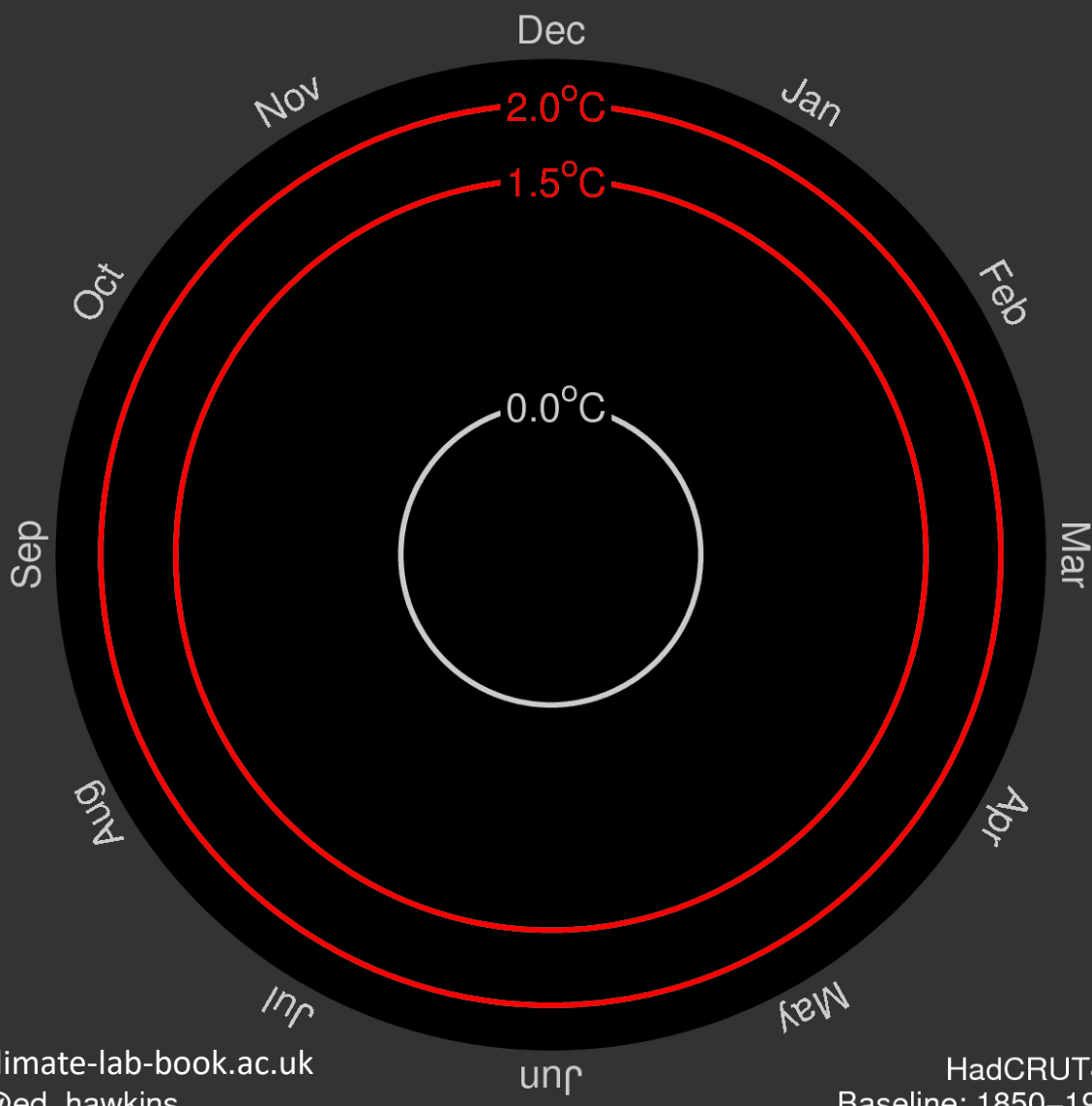


Is global warming spiraling out of control?

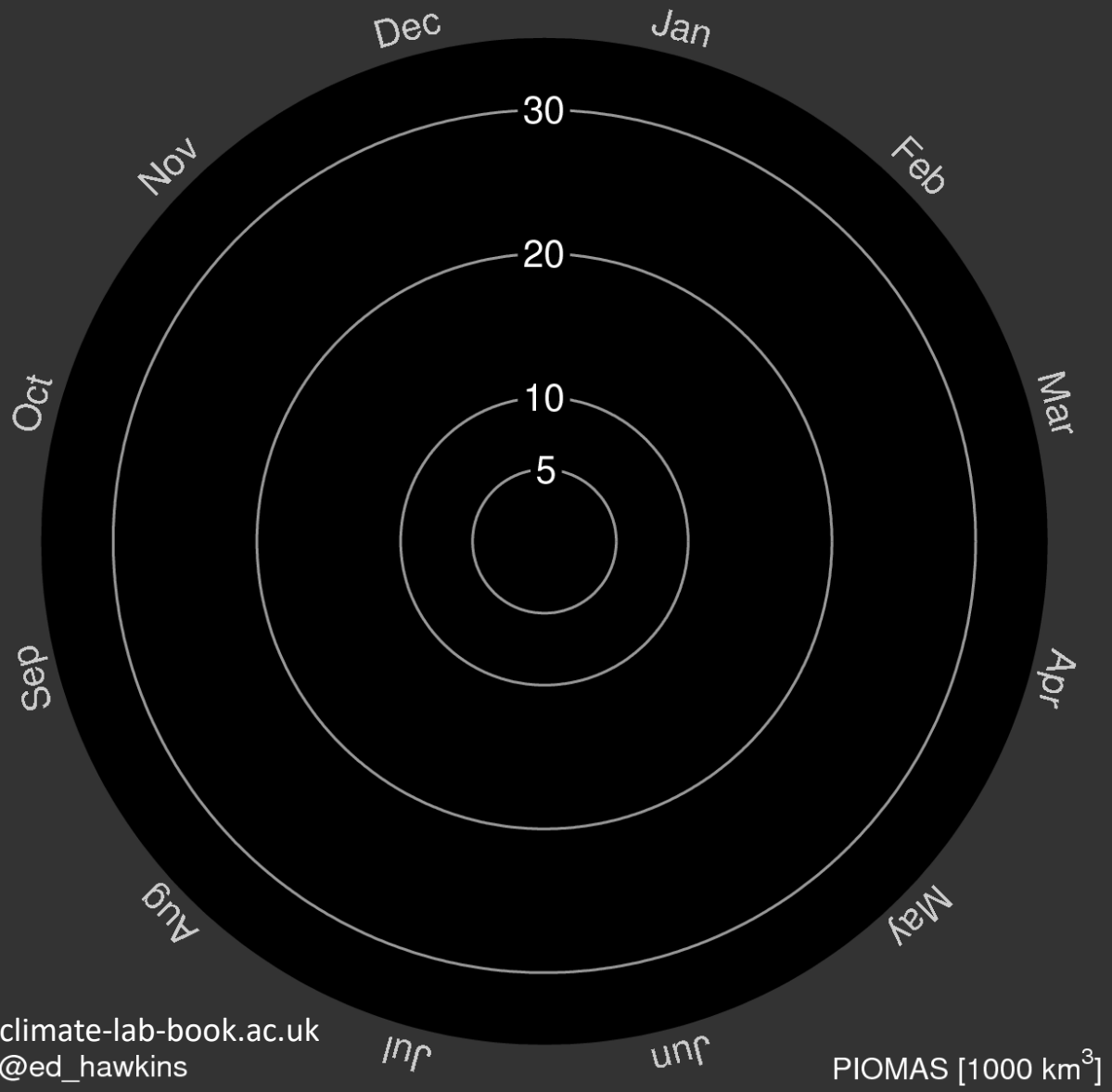
Global temperature change (1850–2017)



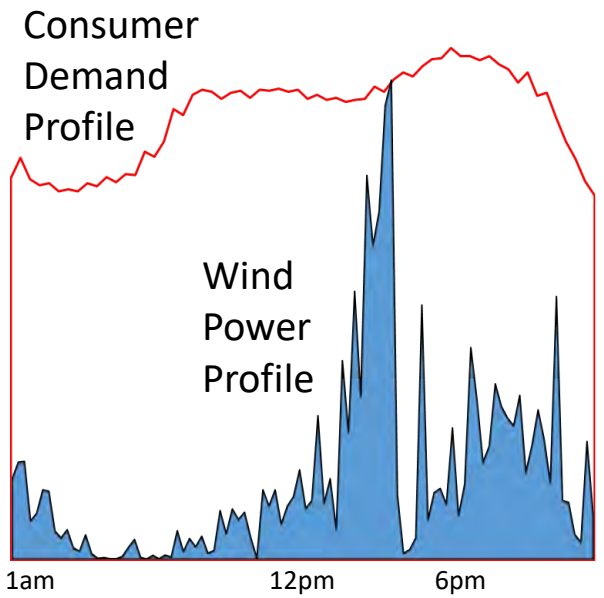
climate-lab-book.ac.uk
@ed_hawkins

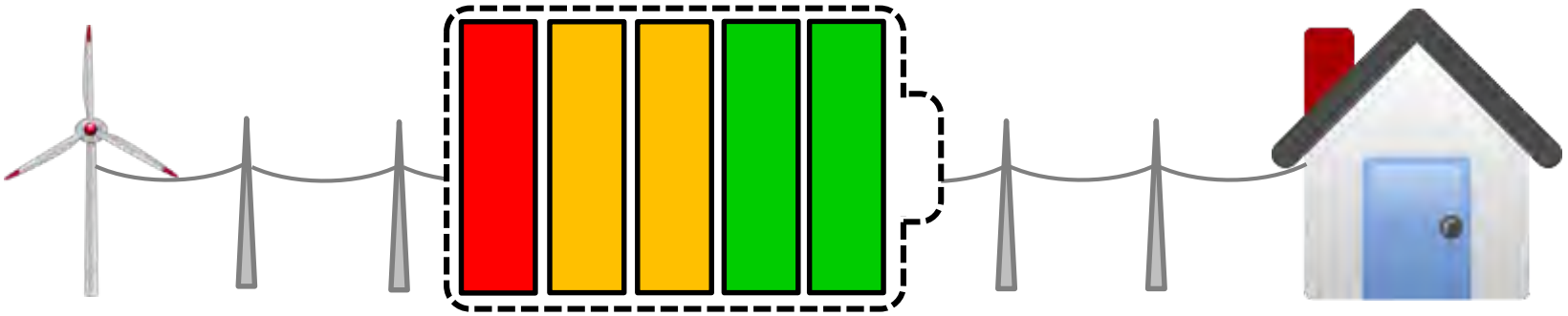
HadCRUT4.6
Baseline: 1850–1900

Is our climate circling the drain?



Renewable Energy Economy Batteries Not Included



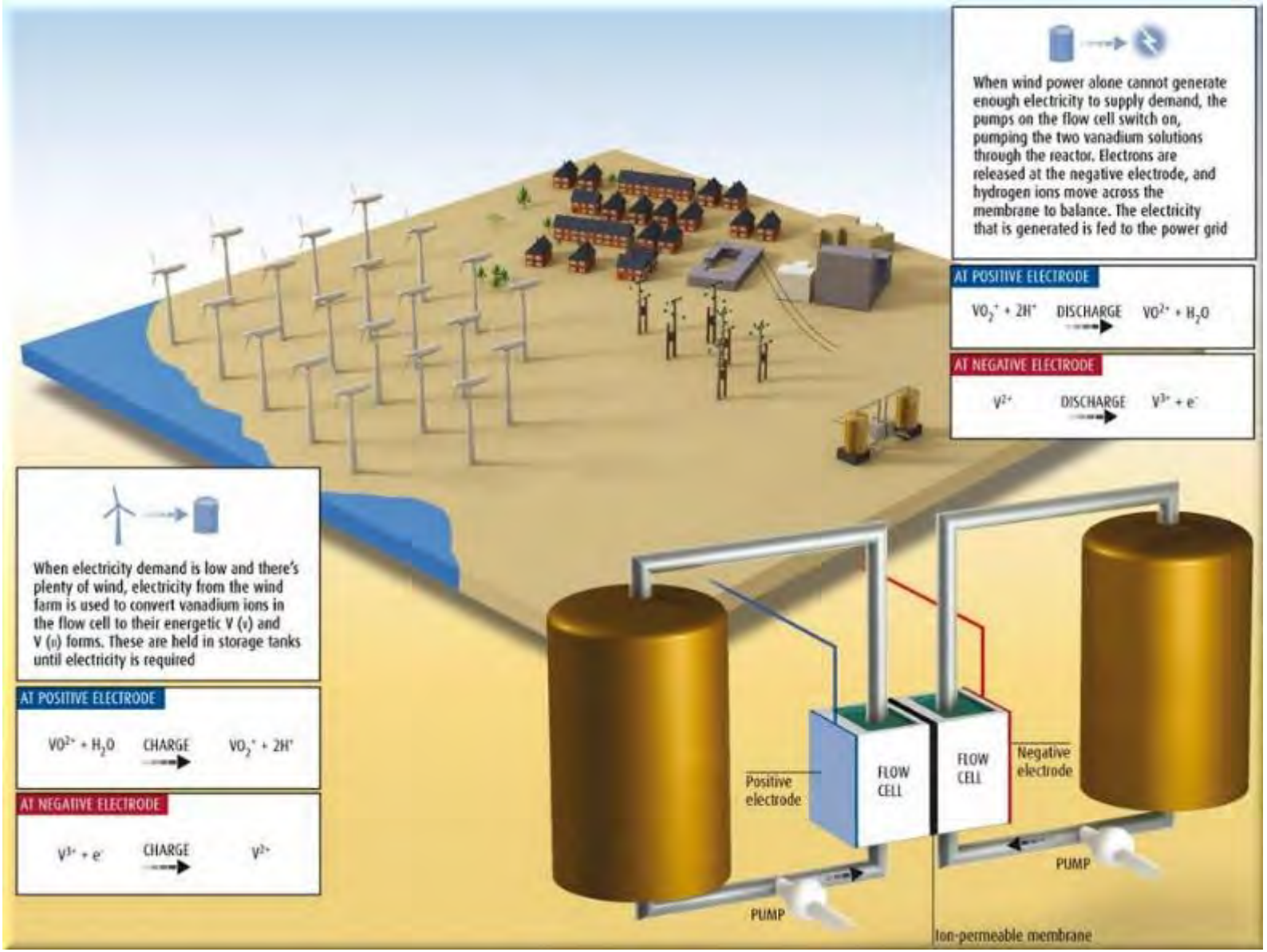


Renewable Energy Economy Not Just Mega-Hype

100MW - 129MWh
Or 1.3 hours at full capacity

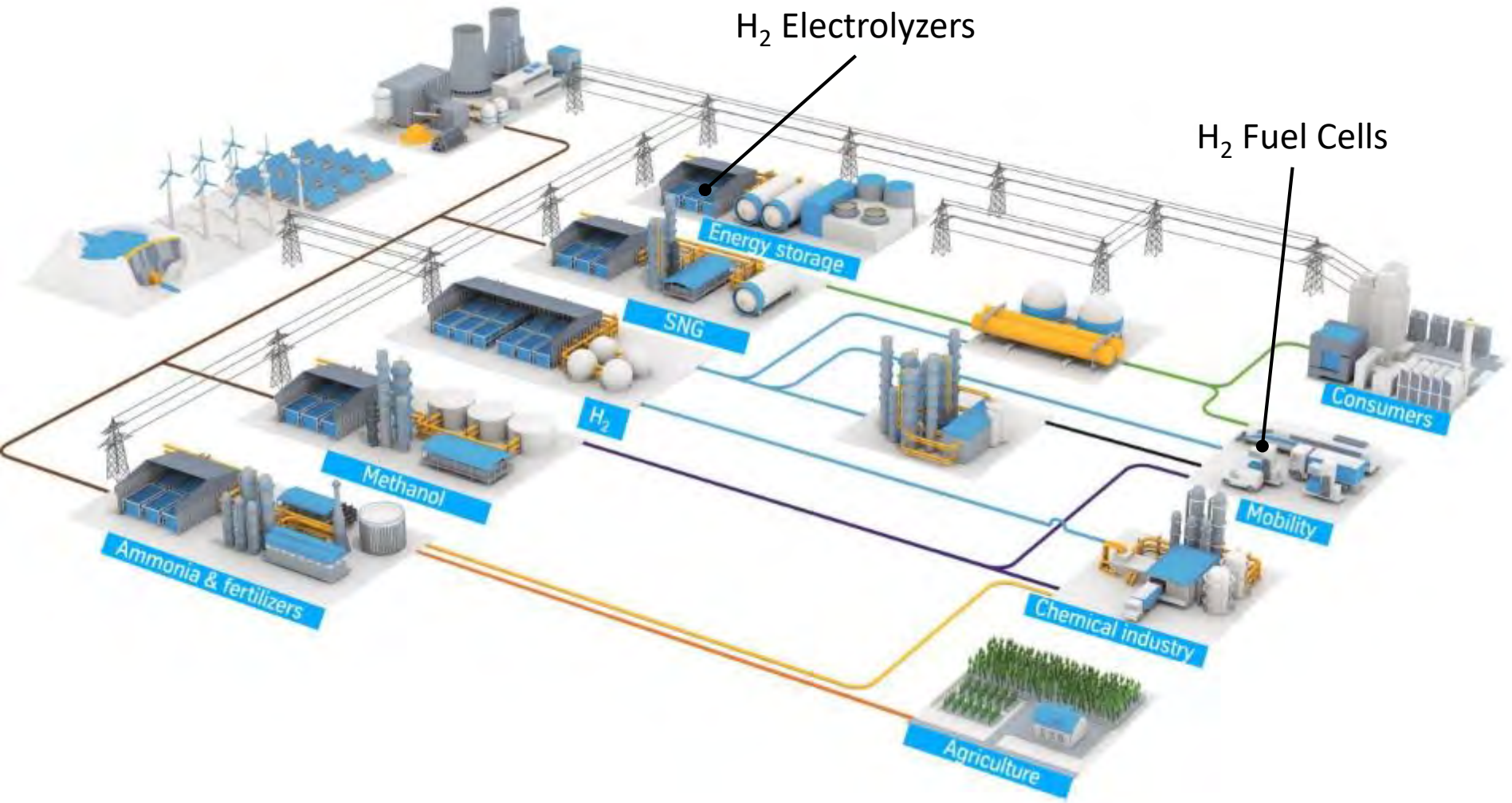
https://cleantechnica.com/2018/08/29/

Renewable Energy Economy Go With the Flow



Weber et al. J App Electrochem (2011)

Renewable Energy Economy Hydrogen Economy



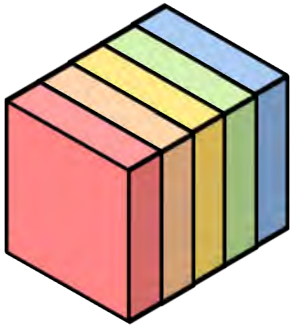
https://www.thyssenkrupp-uhde-chlorine-engineers.com/en/products/water-electrolysis-hydrogen-production/power-to-gas/

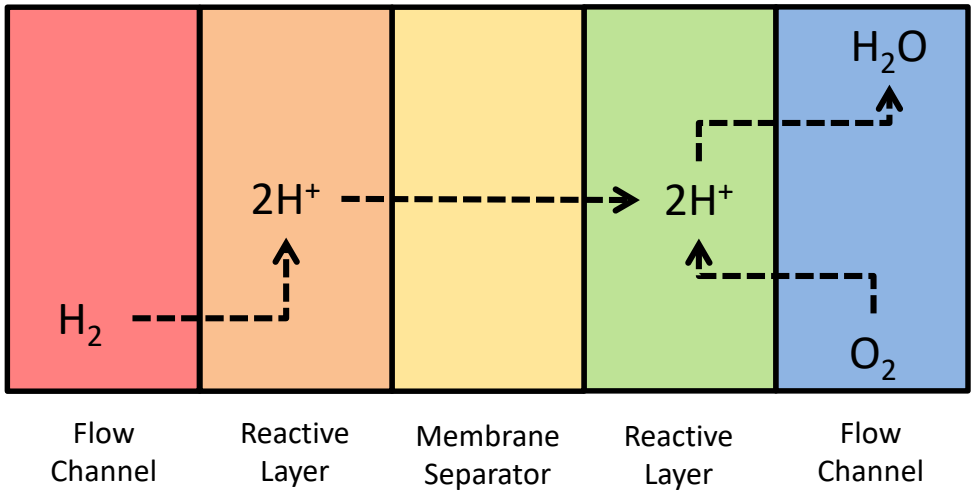
Renewable Energy Economy Turning Water into Wine

https://www.hydrogenics.com/technology-resources/media-downloads-table/

Porous Electrodes

Cells consist of several layers, each with its own function, and reactants (e.g. ions, electrons) must travel **through** each layer



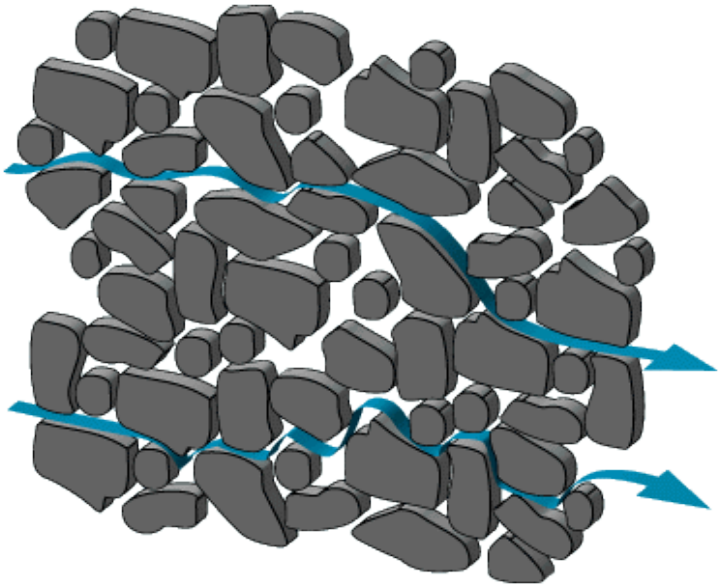


Each layer in the cell presents some sort of **resistance** to the transport of reactive species

Porous materials are a "necessary evil":

- The solid structure conducts electrons
- The void phase allows chemical delivery
- The void-solid interface support reactions

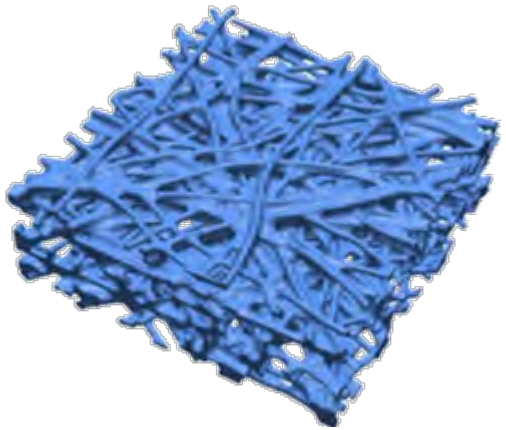
But each hinders the other

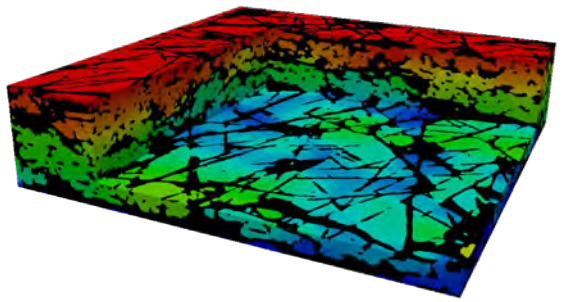


Outline for Remainder of Talk

Part 1: Volumetric Image Analysis

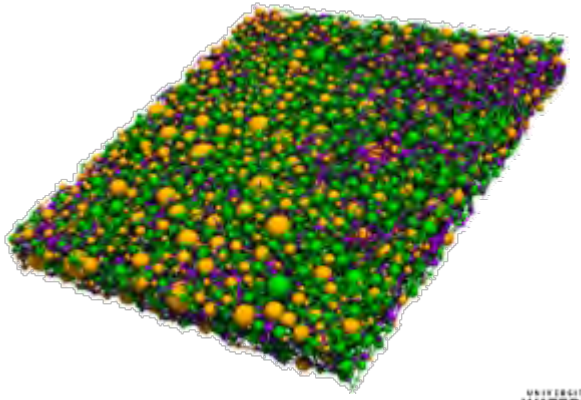
- Introduce the idea of a ‘volumetric image’
  - How they are obtained
- Describe what they are used for
  - Quantitative image analysis
  - Direct numerical simulations
  - Why they are a pain





Part 2: Pore Network Modeling

- Introduce pore network modeling
  - What it means
  - How it helps
- Case Study: Li-ion battery
- Next steps



Part 1

VOLUMETRIC IMAGES

X-Ray Computed Tomography Lab Size Magic Box

Apply some magic

Sample goes in

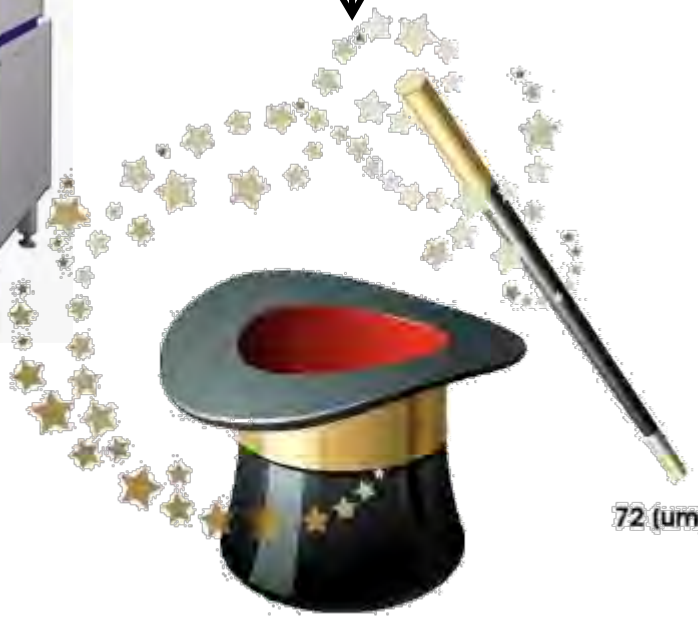


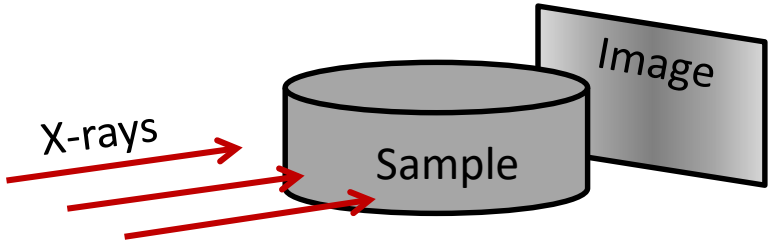
Image comes out

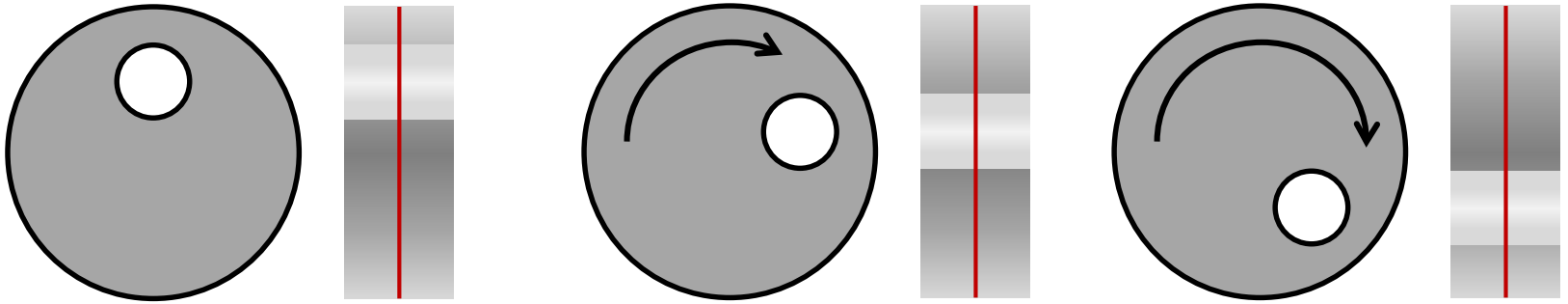
X-Ray Tomography We Can See Inside the Pores !

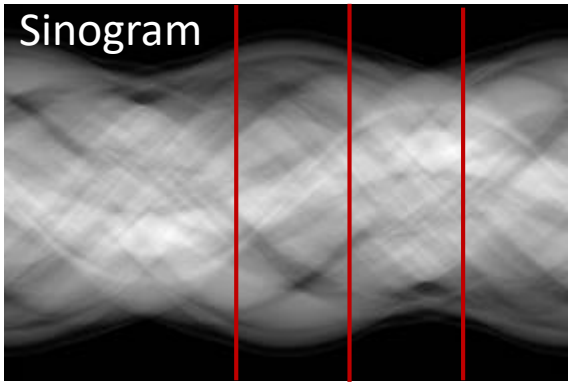
Tomography is more commonly known as a “CAT” scan, or “CT” Scan

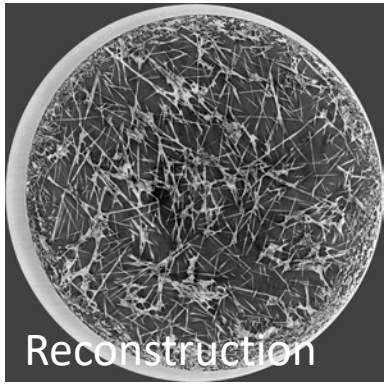
An X-ray image has dark spots where X-rays are attenuated by a dense material…

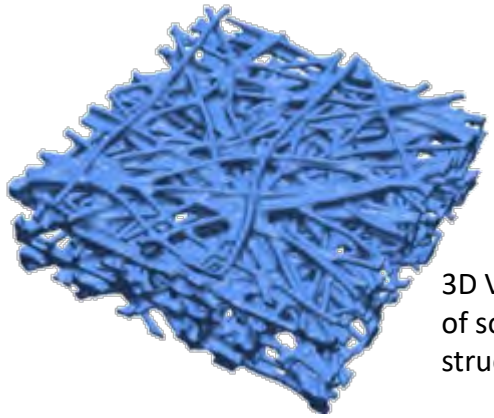
…or *MORE* material







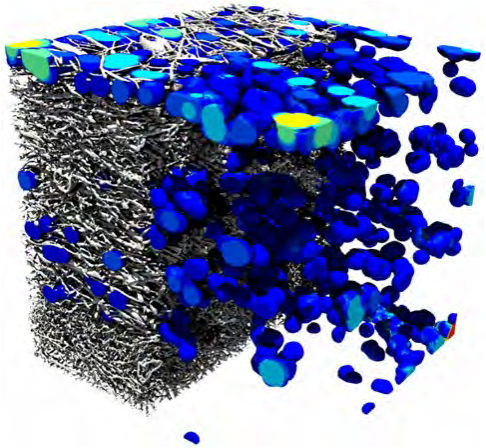


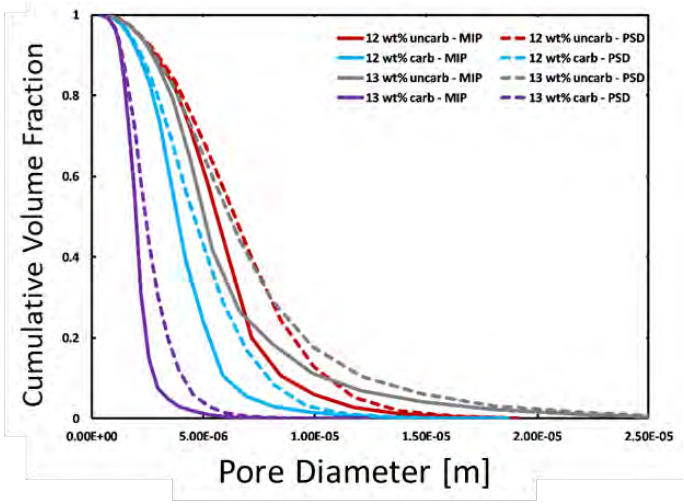


3D Voxel image of solid and void structure

Quantitative Image Analysis In-Silico Experiments

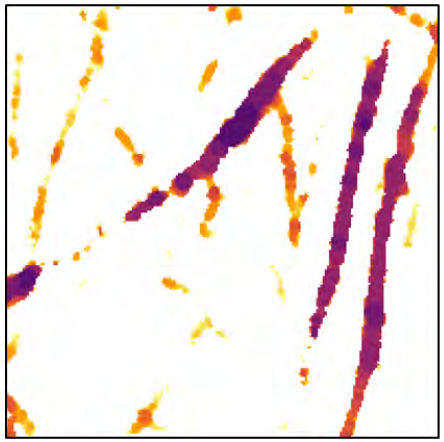
Cumulative pore size curves

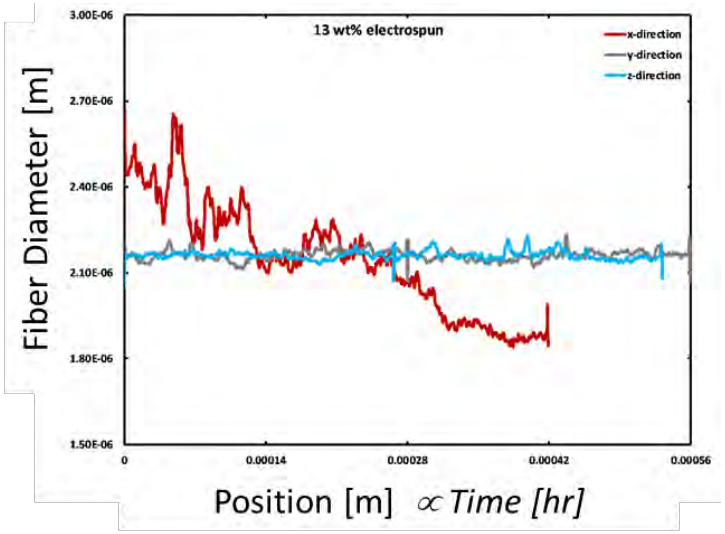




Porespy

Spatial distribution of fiber diameters

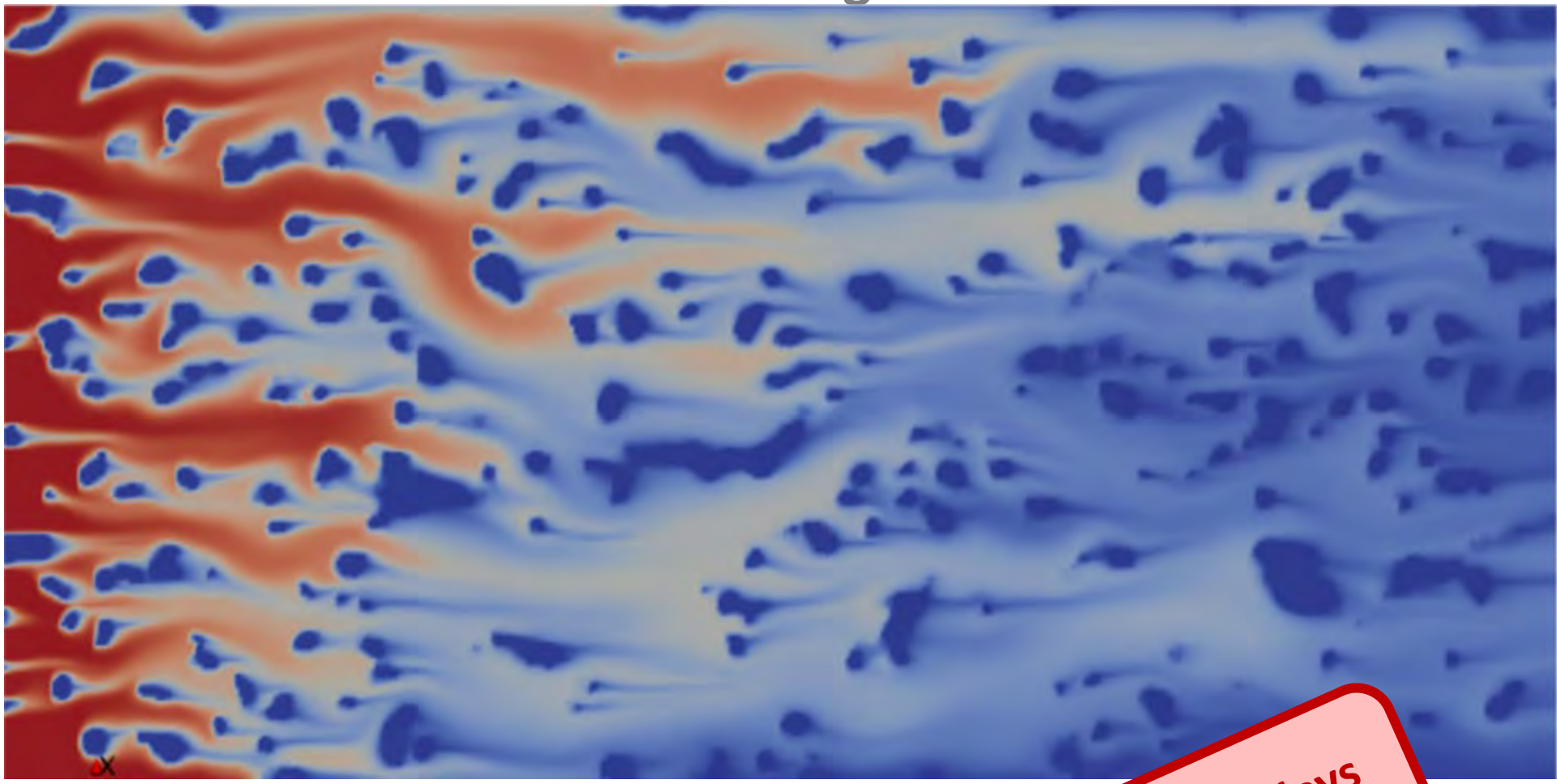




Self-proclaimed mission statement:

"In a perfect world, this journal should NOT exist, but software developers must justify their existance by counting publications just like everyone else"

Direct Numerical Simulation Engineers' Dream Date



- Each voxel* in the image is a computational unknown
- Fluid flow is solved using Lattice-Boltzmann method
- Fiber surfaces are reactive (consuming 'red stuff')
- Diffusion/reaction is solved on top of flow field

Takes 1+ days to complete!

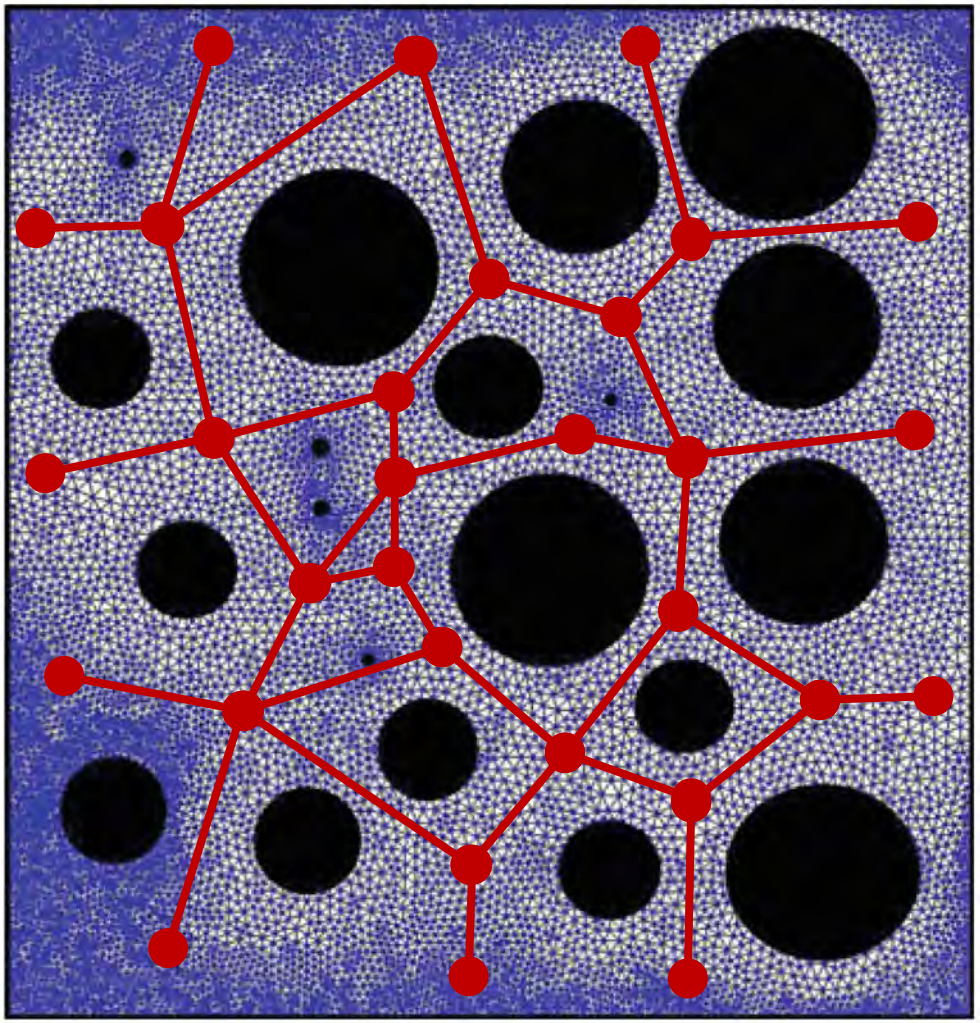
* A voxel is a 3D pixel

Part 2

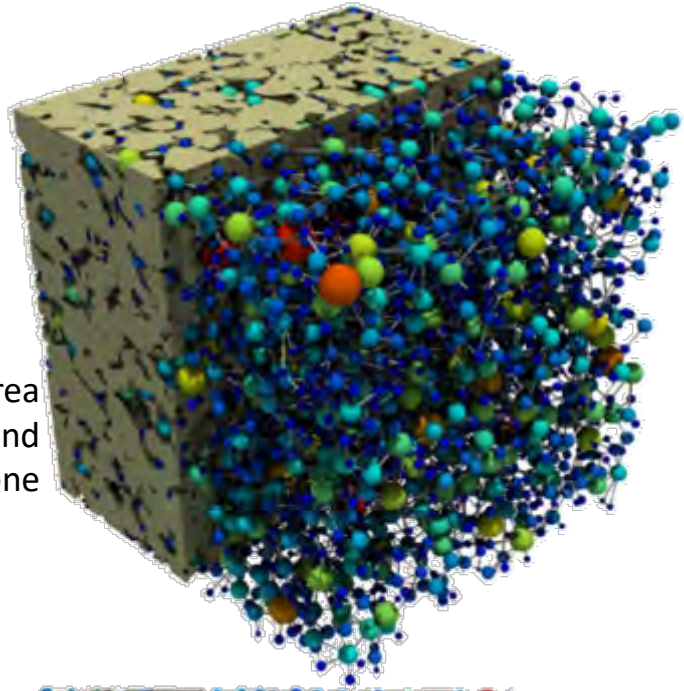
PORE NETWORK MODELING

Pore Network Modeling Abstracting Pores and Throats

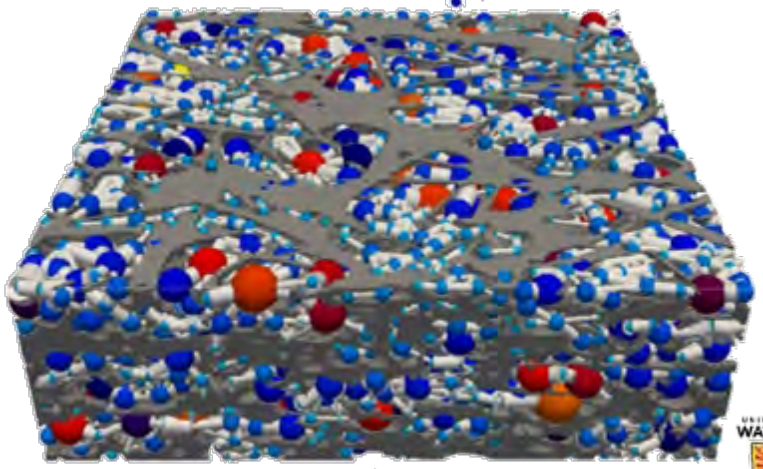
Pore network models abstract the domain as pores (balls) and throats (sticks)



10^4 DoF → 10^1 DoF

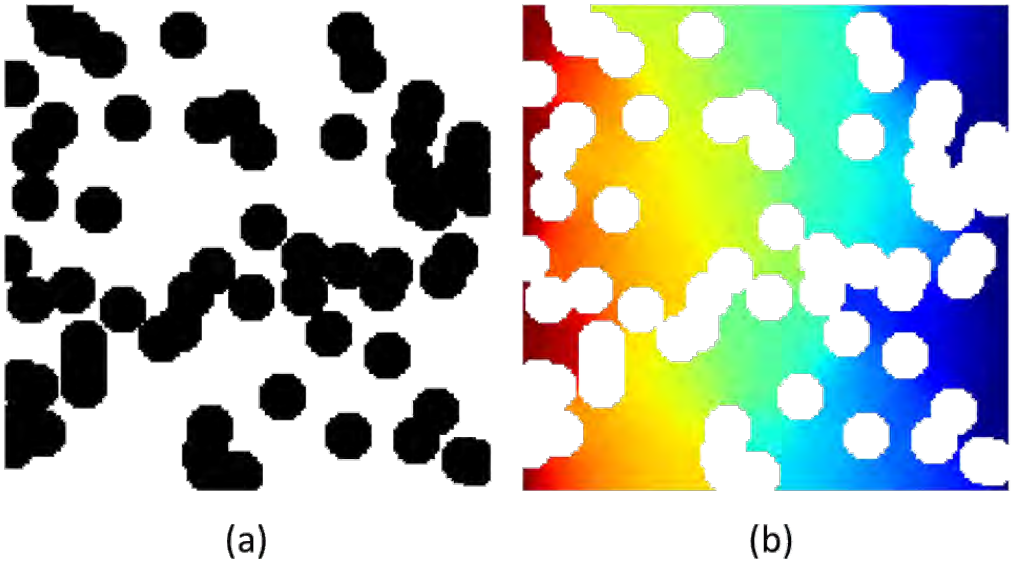


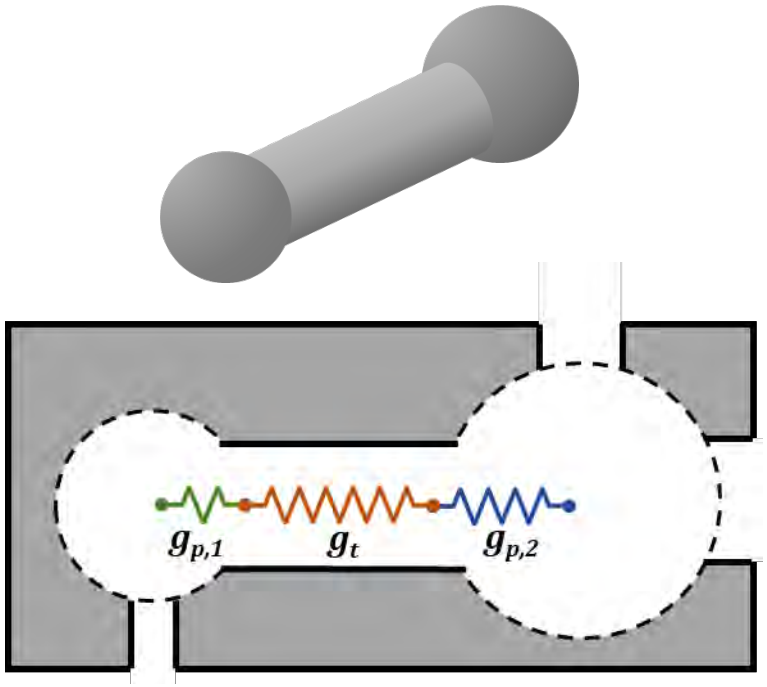
Berea Sand Stone



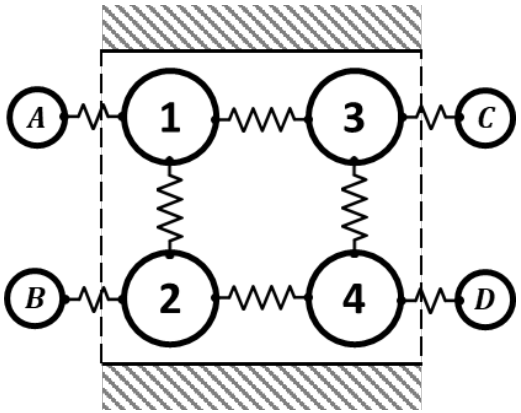
Gas Distribution Layer

Pore Network Modeling Extracting Size and Connectivity





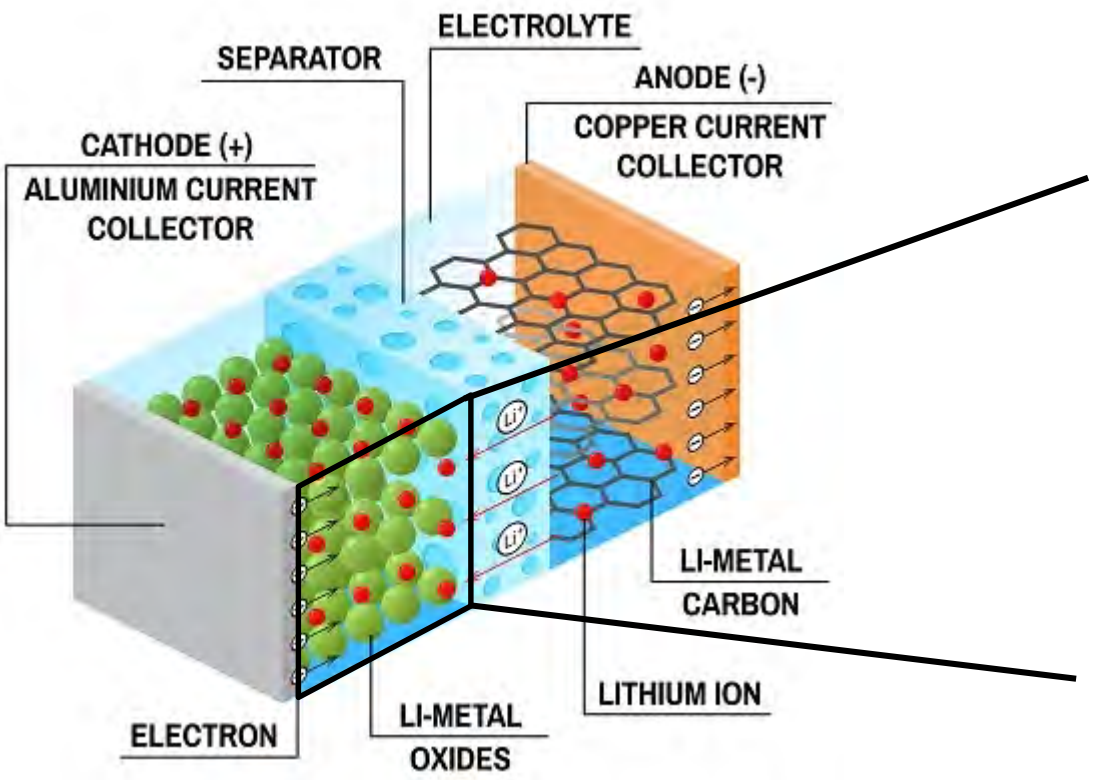
$$Q = \frac{\pi R^4}{8\mu L}\Delta P = g\Delta P \longrightarrow I = \frac{1}{R}\Delta V$$

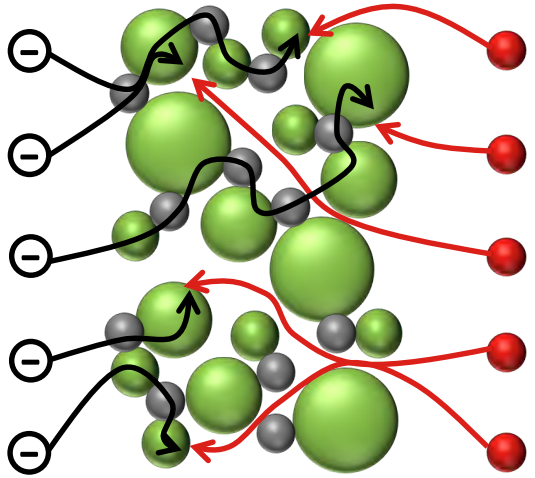


Gostick, Physical Review E (2017)

Case Study Li-Ion Batteries

Recall the 'layered' structure of electrochemical cells:

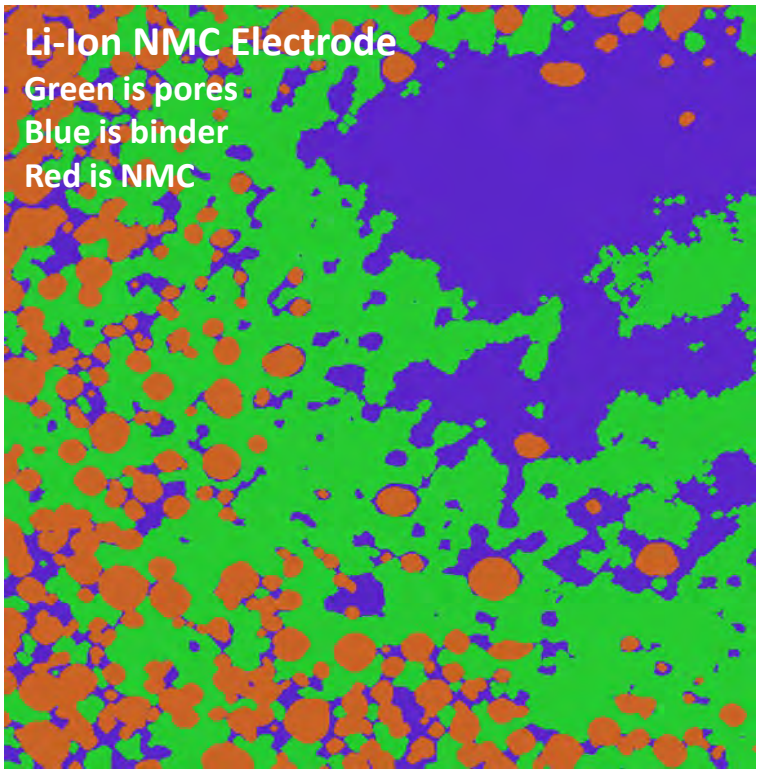




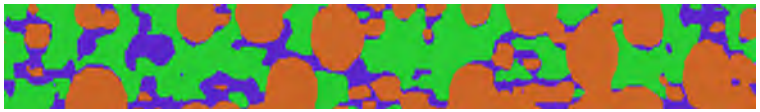
Transport in a Li-ion Electrode:

- Active solid particles (ion storage) → More is better
- Binder particles (electron conduction) → More is better
- Liquid filled void (ion transport) → More is better
- Liquid-Solid Interface (ion insert themselves into active material) → More is better

Li-Ion Battery Materials Computational Overload



Top view and edge view

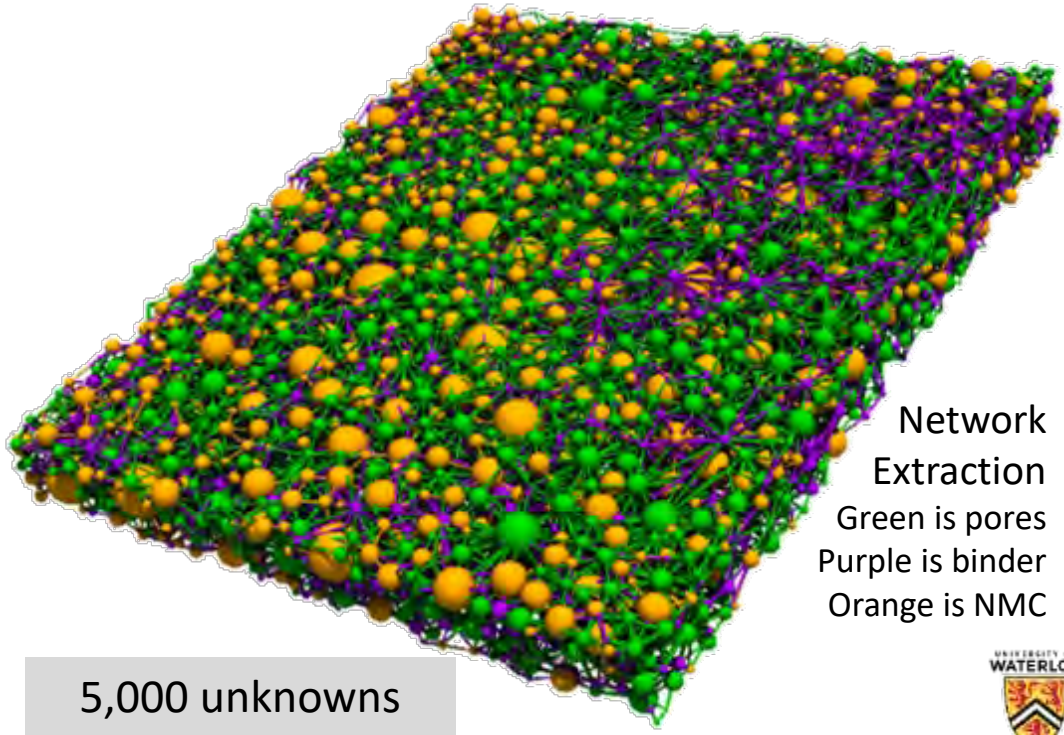


500 x 500 x 200 = 50 million unknowns

- Coupled Multiphysics*
  - Diffusion-Migration (Nernst-Plank)
  - Non-linear kinetics (Bulter-Volmer)
  - Heat and electron conduction (Fourier and Ohm's law)
- Transient!
  - All of the above, multiplied 1000x for each time step

Pore Network Modeling:

- "…because the only option is the best option"©



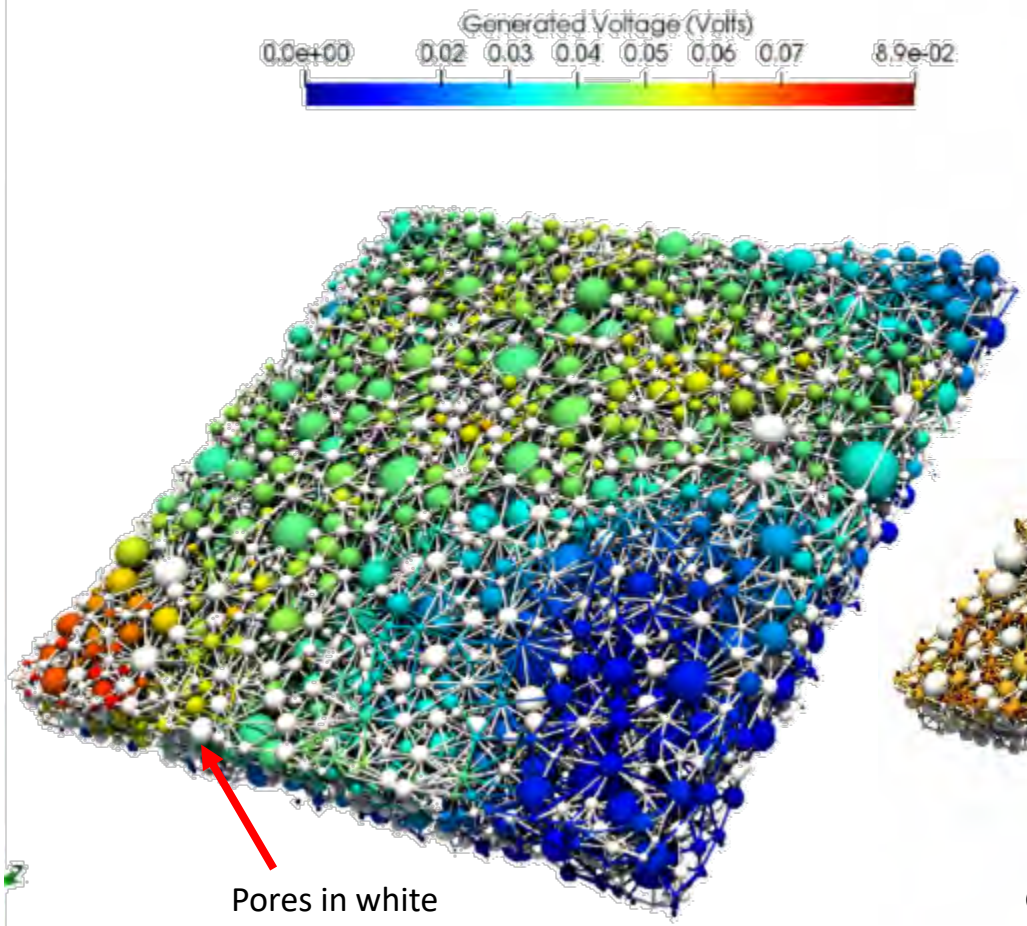
Network Extraction
Green is pores
Purple is binder
Orange is NMC

5,000 unknowns

Li-Ion Battery Materials Reduced Order Modeling

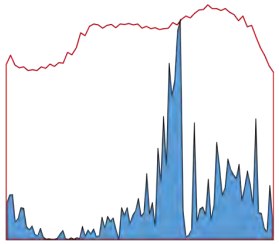
Coupled Ion and Electron Transport

- Obtained in a matter of <u>seconds</u>

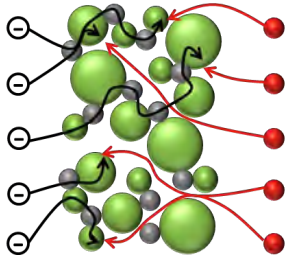


Summary

- Electrochemical energy storage is currently the leading candidate
  - Is essential for enabling the ‘renewable energy economy’

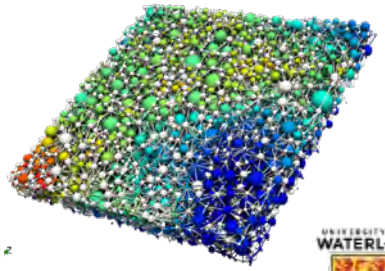


- Pore structure of electrodes is crucial for performance
  - Researchers use trial and error to create novel materials
  - Do post-hoc analysis to understand results



- Volumetric imaging has become quite common
  - Lab-scale tomography scanners are widely available
  - Tools to extract ‘value’ from large images are needed

- Pore network modeling offers a promising path
  - Computationally feasible means of studying the structure-performance relationship



Acknowledgements

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Zohaib Khan
Mehrez Agnaou
Missing: Amin Sadeghi

The End

TIME FOR QUESTIONS?

Li-Battery Materials PNM and DNS Comparison