CHONGQING UNIVERSITY

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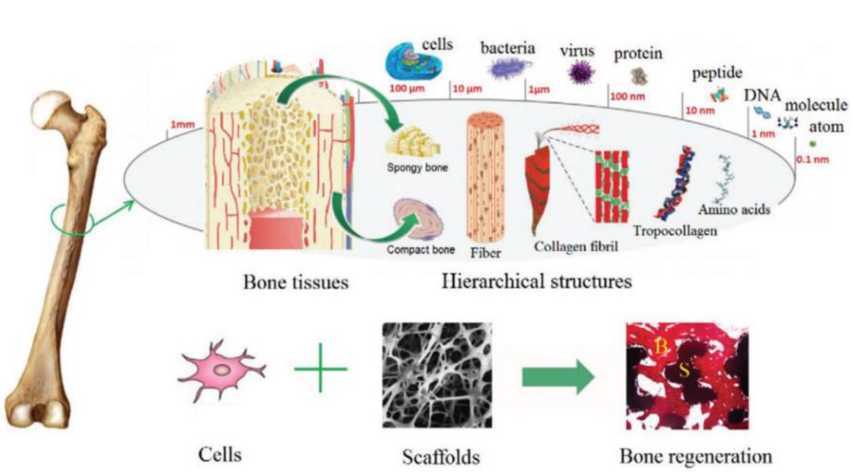
Flow and Transport in Multiscale Pore Structures: Model Development and Simulations

Chao-Zhong Qin, Bowen Shi, Han Jiang, Xingyuan Zhao (Chongqing University, China)
Bo Guo (University of Arizona, USA)

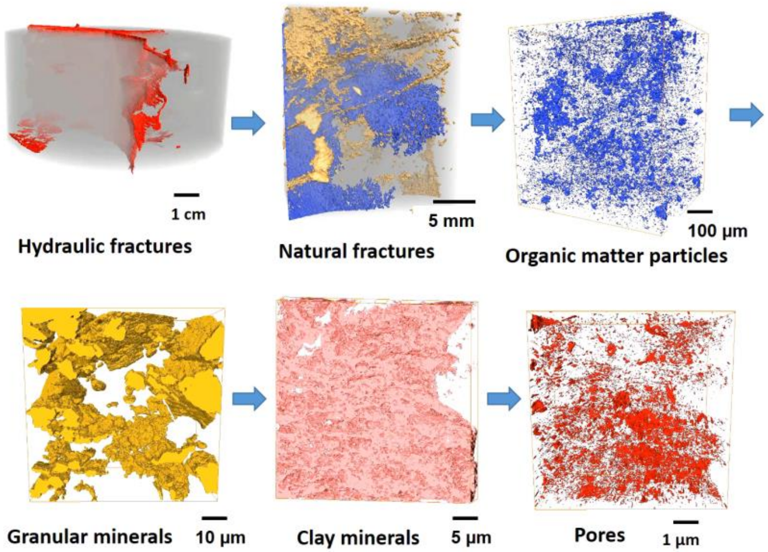
Outline

1. Multiscale porous materials and research challenges
2. Two hybrid numerical models for multiscale digital rocks
3. Predictions of single-phase and two-phase flow parameters
4. Conclusions and outlook

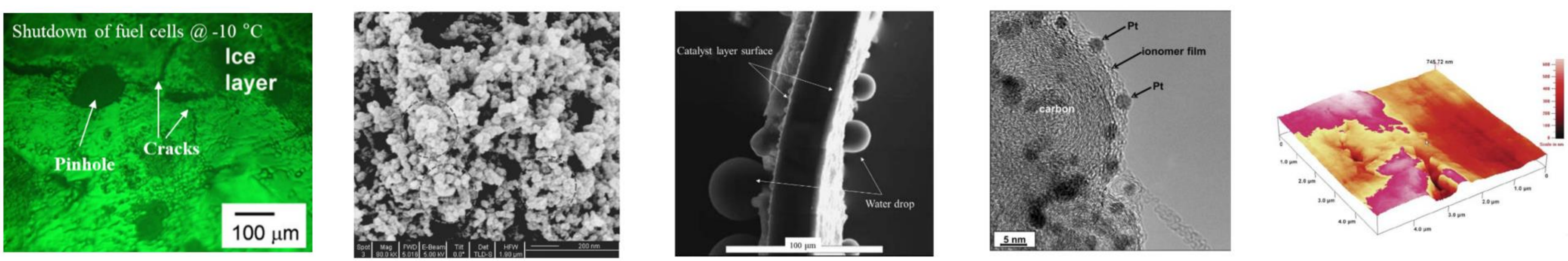
Multiscale porous materials across different applications



Hierarchical pore structure of bone tissue (*Adv. Funct. Mater. 2021, 31, 2010609*)



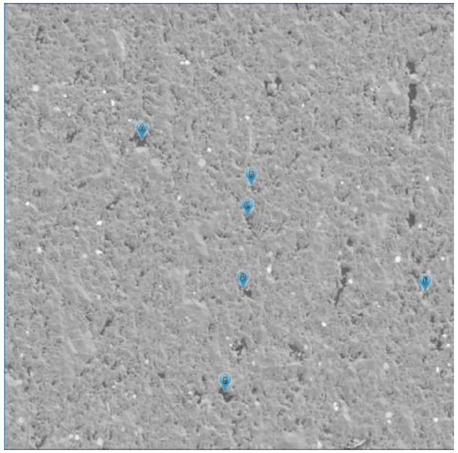
Hierarchical pore structures of shale



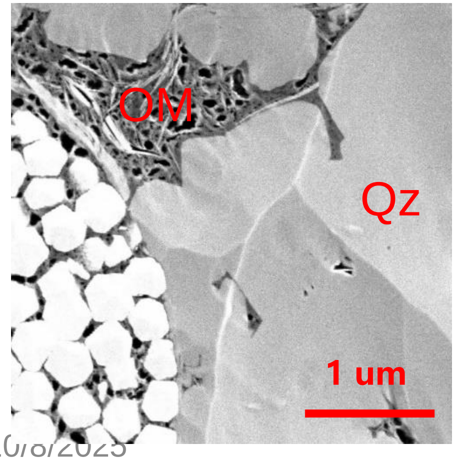
Hierarchical pore structure of catalysts (*Electrochem. Energ. Rev. 2023, 6, 13*)

Research challenges for flow and transport

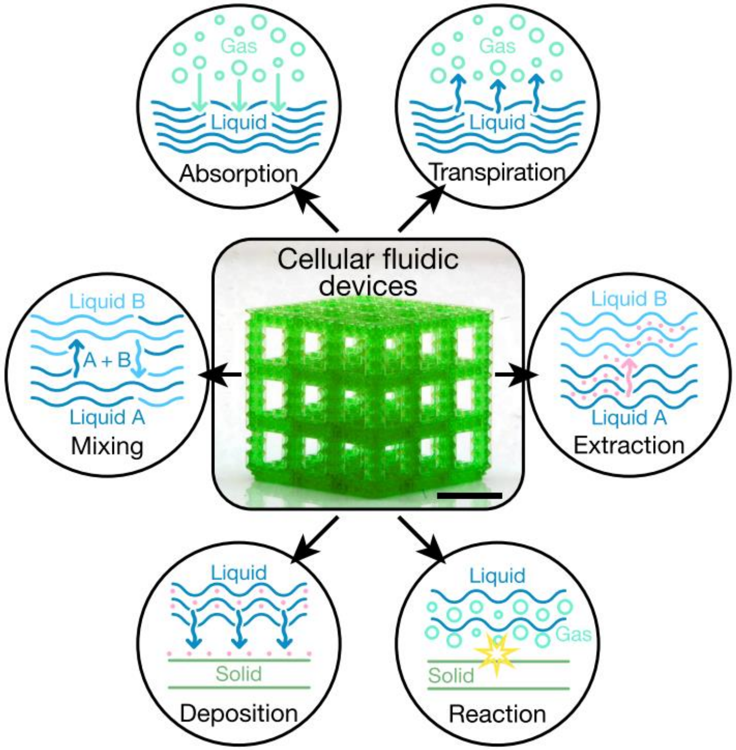
- How do **multiscale pore structures** regulate flow and transport?
- The role of **wettability** in flow and transport, and how to **control wettability**?



MAPS of shale



Combine wettability and multiscale pore structures?



Nature, 2021

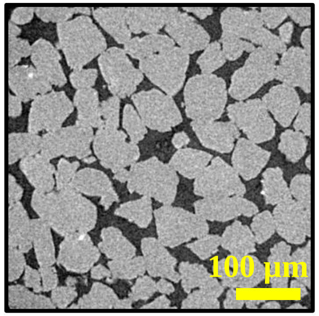
Outline

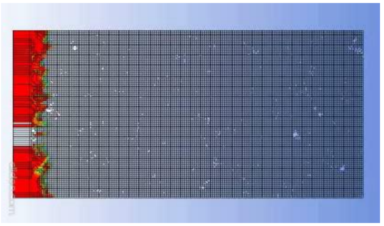
1. **Multiscale porous materials and research challenges**
2. **Two hybrid numerical models for multiscale digital rocks**
3. **Predictions of single-phase and two-phase flow parameters**
4. **Conclusions and outlook**

Characterization of pore structures
Material properties
Hybrid numerical models
} Predict flow and transport processes

Digital Core Analysis (DCA) – multiscale pore structures

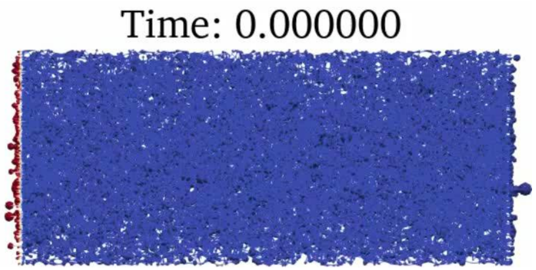
Nubian sandstone





VOF modeling of water imbibition, $100 \times 100 \times 200$ image

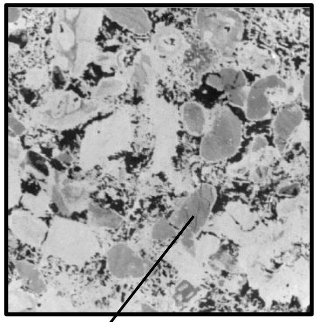
(*Qin et al., AWR, 2021*)



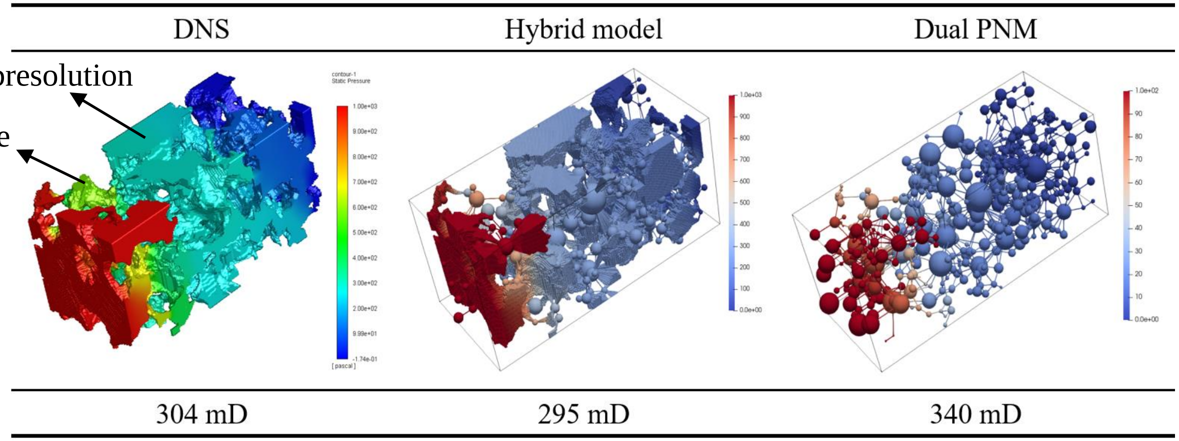
$900 \times 900 \times 2000$ image

Dynamic pore-network modeling of cocurrent spontaneous imbibition

Estaillades carbonate



Subresolution microporosity

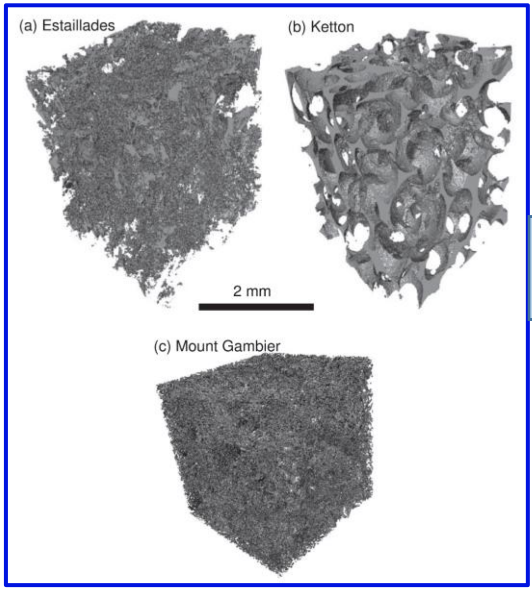


(*Qin et al., TiPM, 2025)*

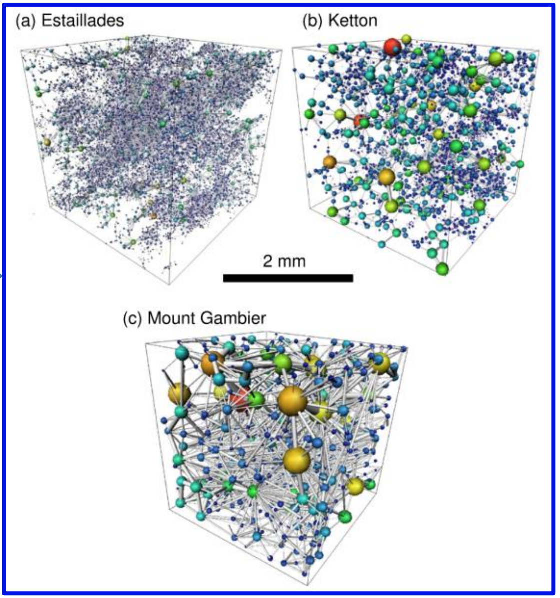
Pore-network models – between DNS and continuum

Flow and transport

- ❑ Quasi-static or dynamic two-phase flow
- ❑ Reactive flow and transport
- ❑ Non-Newtonian fluid flow
- ❑ Mineral precipitation and dissolution
- ❑ And so on.



Extract pore networks



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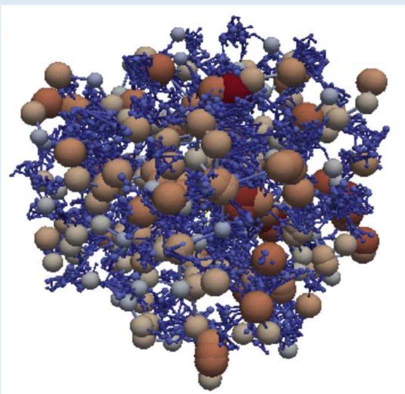
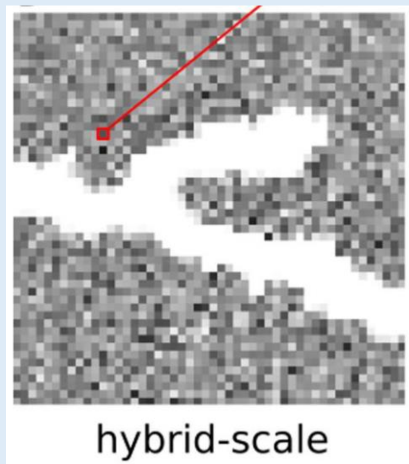
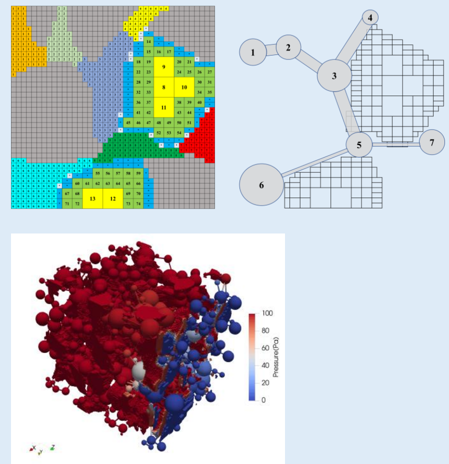
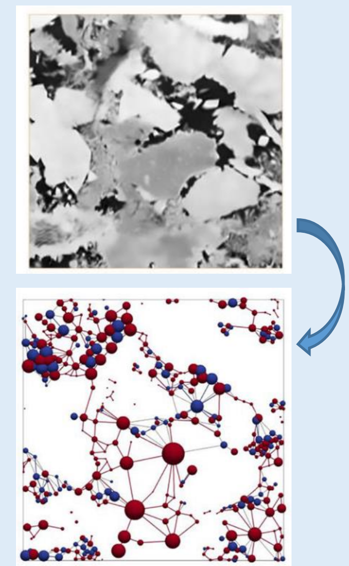
Pore-scale imaging and modelling

Martin J. Blunt [a,*], Branko Bijeljic [a], Hu Dong [b], Oussama Ghar…
Adriana Paluszny [a], Christopher Pentland [a]

[a] Department of Earth Science and Engineering, Imperial College, London SW7 2AZ, UK
[b] iRock Technologies, Suite 1103, Tower A, Oriental Media Center, No. 4 Guanghua Road, Chaoyang Dist…
[c] Department of Petroleum Engineering, Curtin University, 6151 Perth, Australia

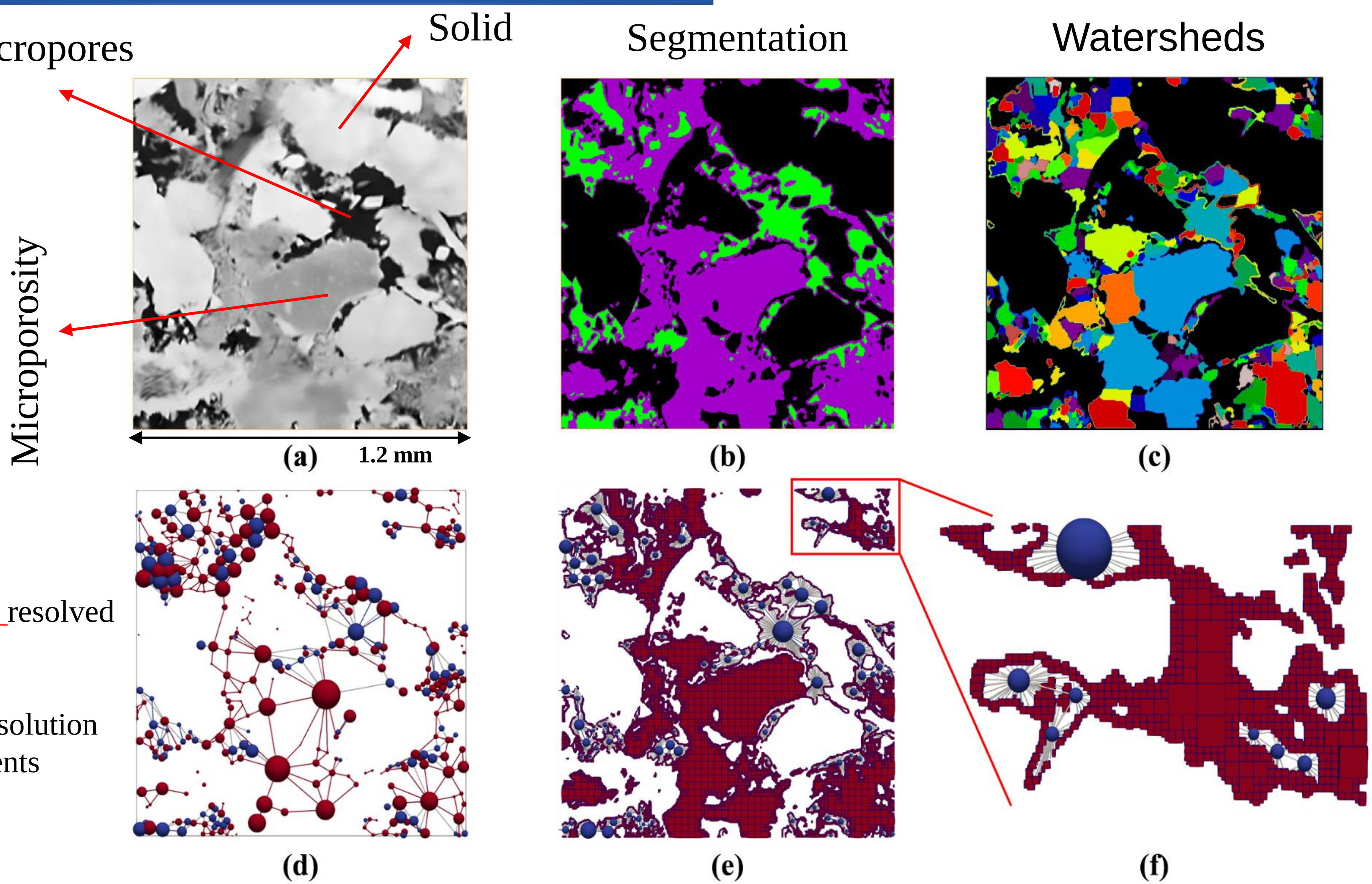
it is difficult to resolve thin wetting layers that control many processes in two and three-phase flow [1,7,8]; this limitation is discussed further at the end of the paper. In the literature to date, the most computationally efficient and successful predictions of multiphase flow come from network modelling, described below.

Numerical models for multiscale porous media

Dual-pore-network model (DPNM)	Micro-continuum model (MCM)	Pore-network-continuum model (PNCM)	Multiscale pore-network model (MPNM)
 Mehmani, 2014	 Soulaine, 2023	 Qin, 2024	

- ❑ The MPNM is most efficient, but **<u>its verification is missing</u>**.
- ❑ The PNCM can **<u>balance efficiency and accuracy</u>**.

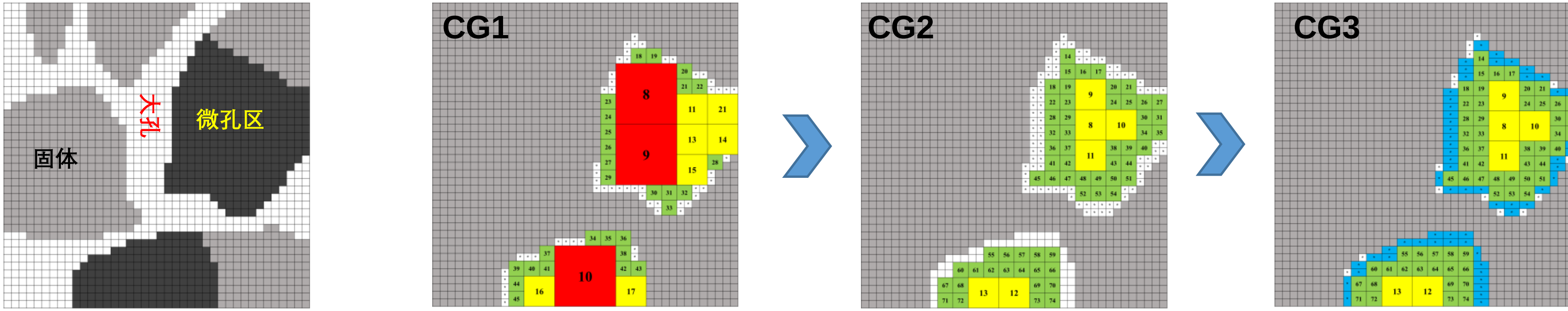
The multiscale pore-network model (MPNM)

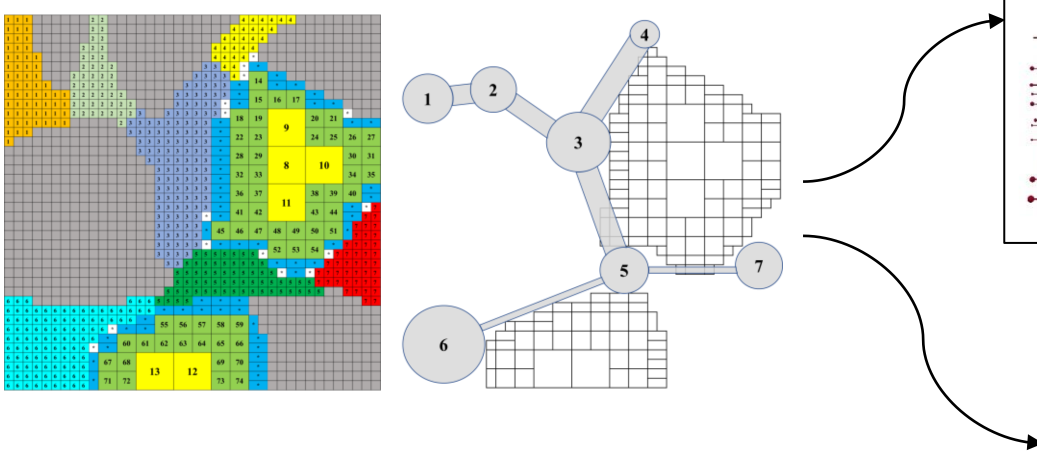


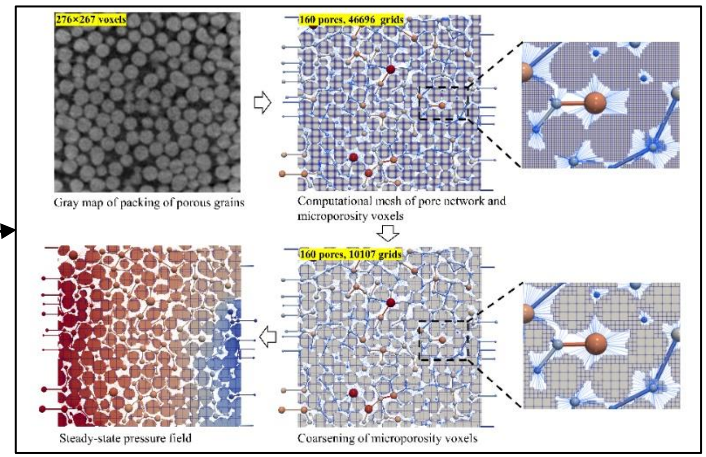
Blue: resolved pores
Red: subresolution elements

1. Modeling of permeability and formation factor of carbonate digital rocks: dual-pore-network and pore-network-continuum models. Transport in Porous Media, 152:37, 2025
2. Modeling of flow and transport in multiscale digital rocks aided by grid coarsening of microporous domains. Journal of Hydrology, 633:131003, 2024

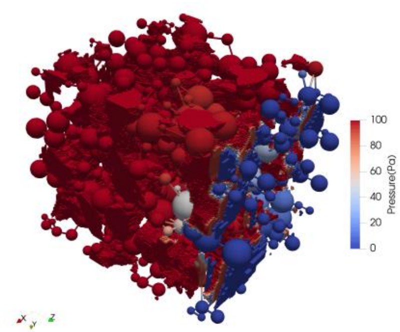
Pore-network-continuum model – coarsening algorithm





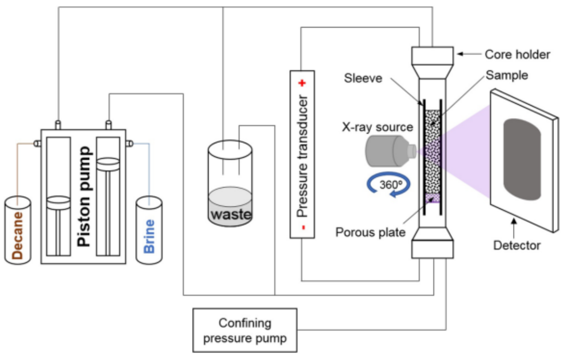


Packing of porous particles

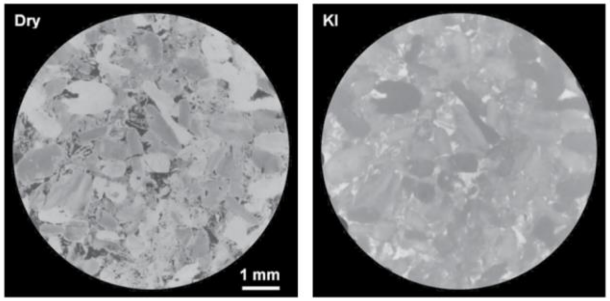


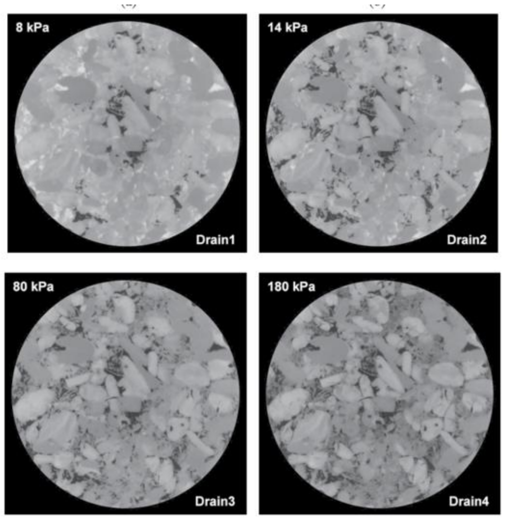
Depressurization process

Characterization of ES6.5 microporosi

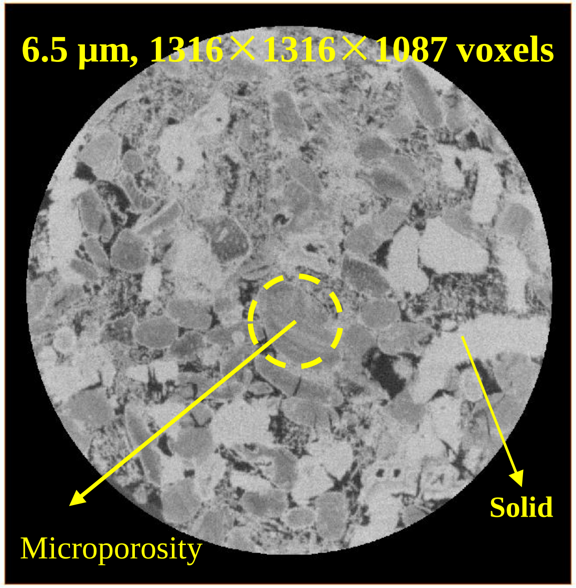


potassium iodide
saturated

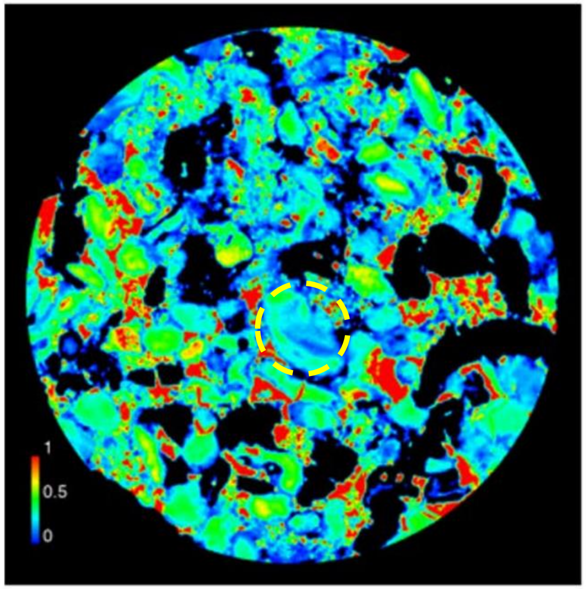




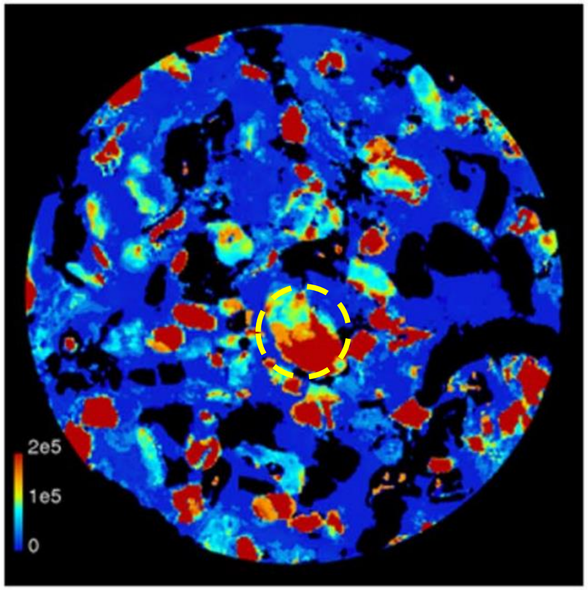
(Wang et al., WRR, 2022)



CT grey-scale map



Porosity map

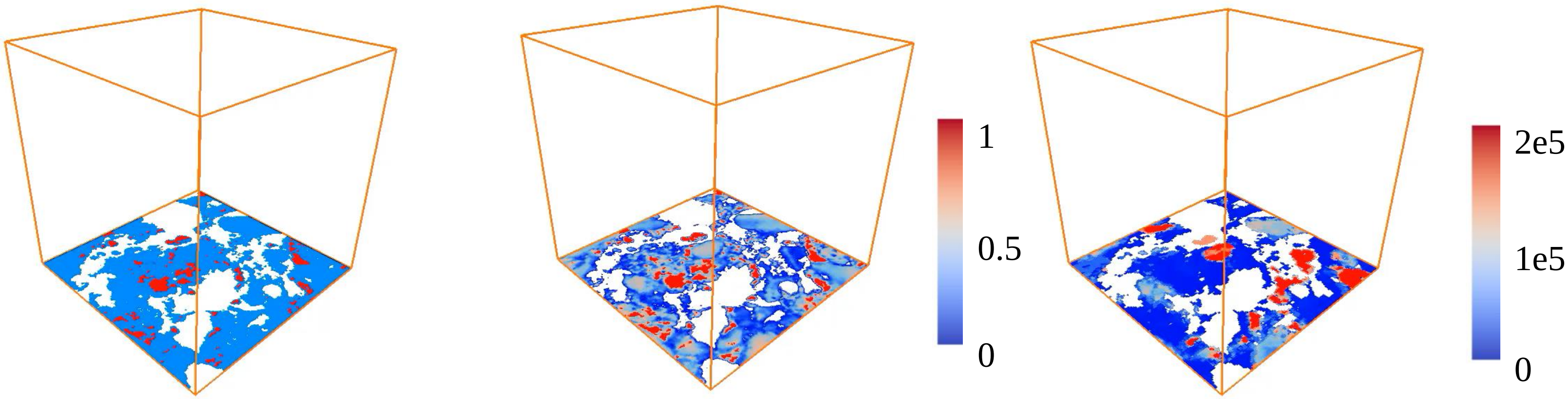


Entry pressure map

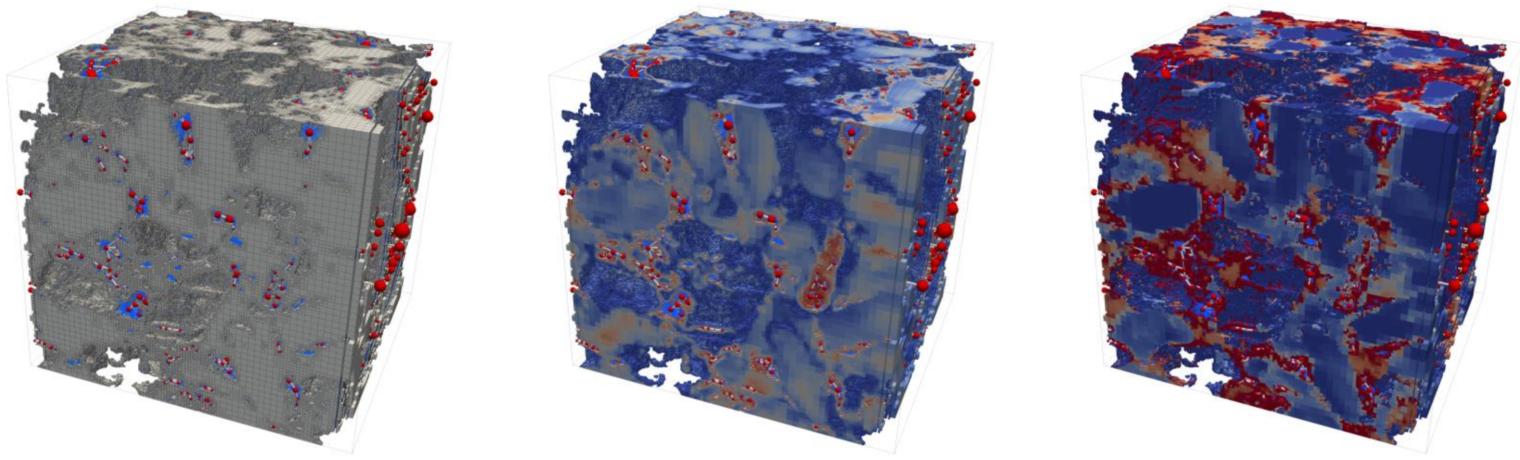
Estaillades carbonate rock： pore structures and mesh

400^3的测试岩心

https://www.digitalrocksportal.org/



Computational mesh for the PNCM modeling



Outline

1. Introduction of multiscale pore-network model
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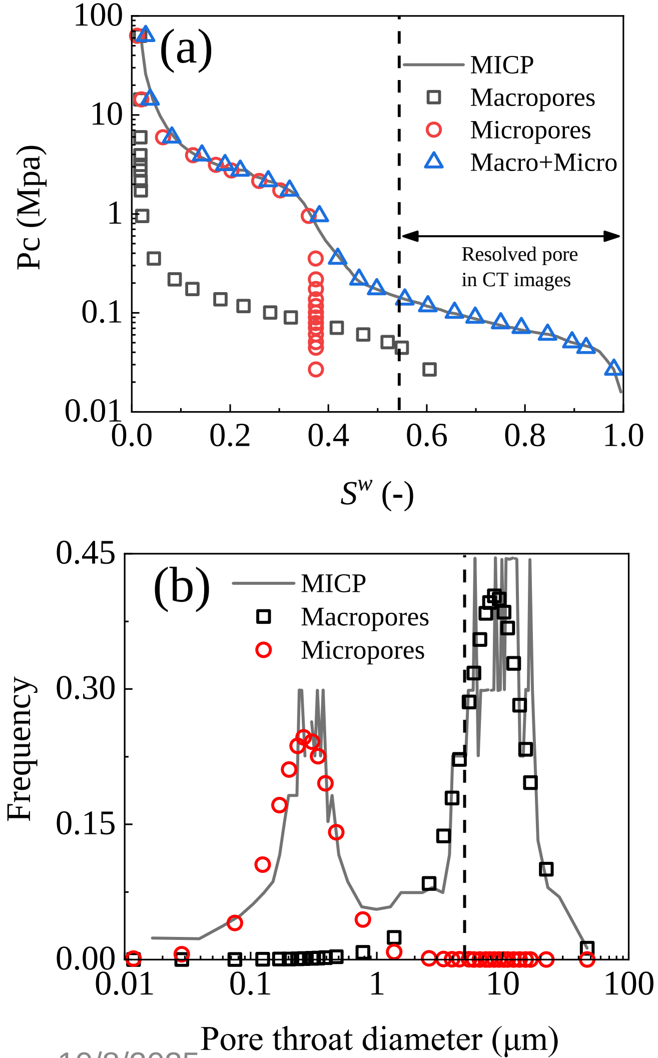
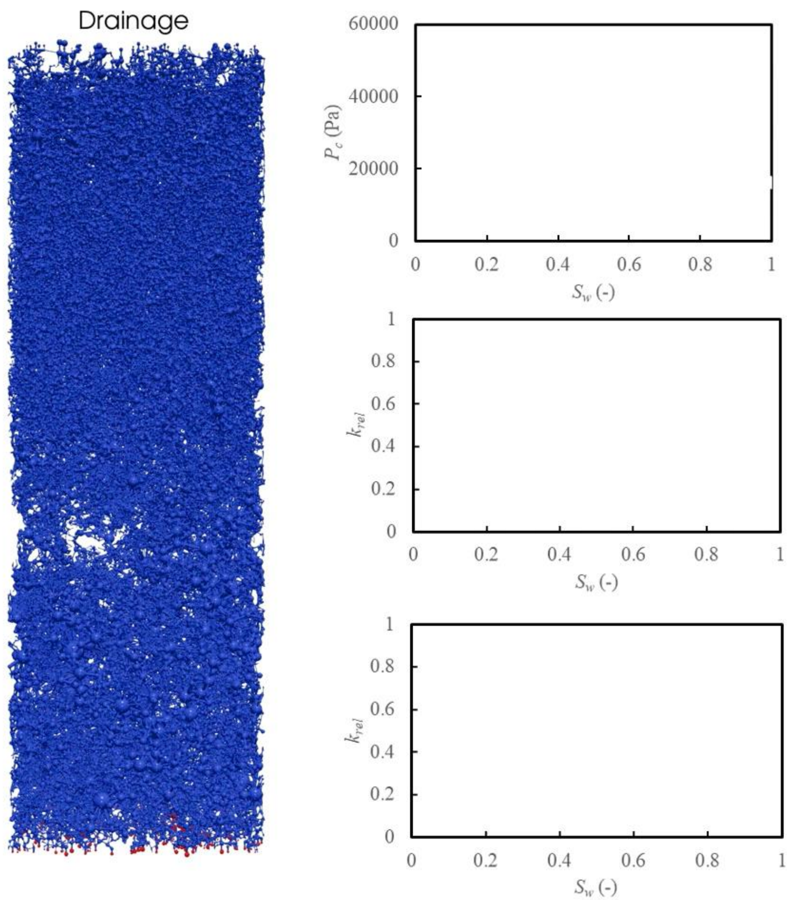
The importance of p^c and k_r

p^c can infer pore-size distributions of porous media

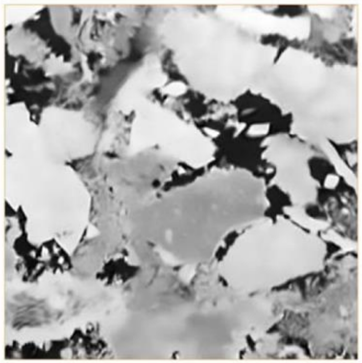


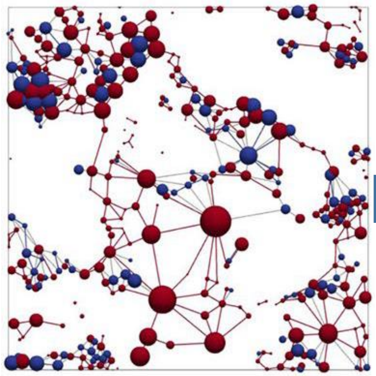
Wetting reservoir

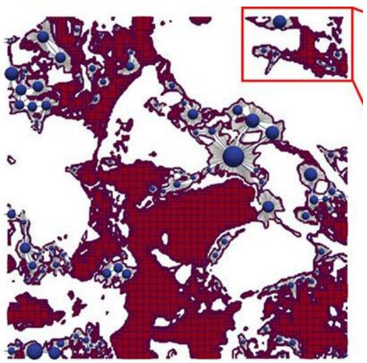


Non-wetting reservoir

The average operation of pore sizes of microporosity in MPNM







① Average based on sphere-assumption

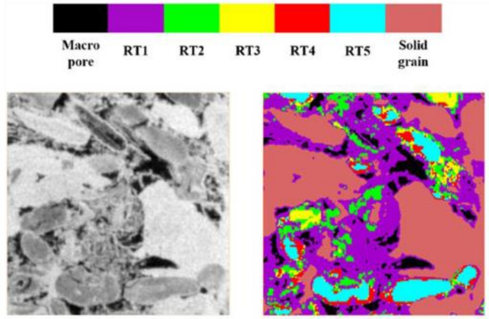
$$\bar{r}_i = \left(\frac{3}{4\pi} \frac{\sum_{k=1}^{N_i} V_k \varepsilon_k}{\sum_{k=1}^{N_i} M_k} \right)^{1/3}$$

$$M_k = V_k \varepsilon_k / \left(4\pi r_k^3 / 3\right)$$

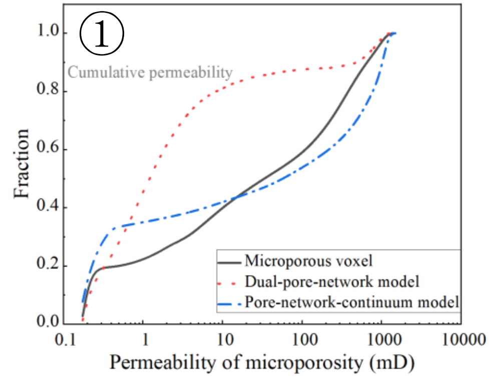
② Average based on voxel-counting

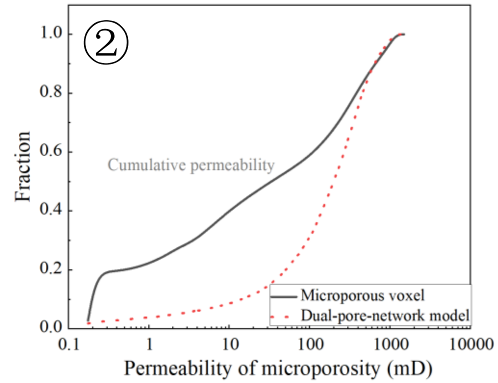
$$\bar{r}_j = \frac{\sum_{k=1}^{N_i} \sum r}{N_i}$$

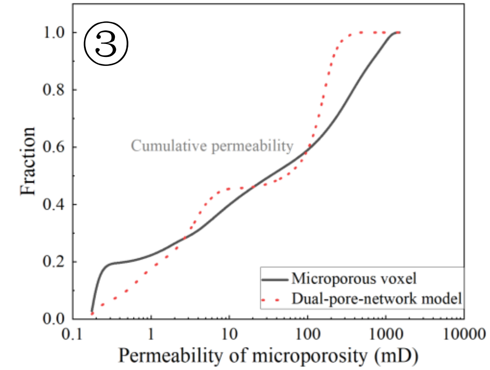
③ Entry-pressure-based sub-rock typing (Wang et al., 2022)



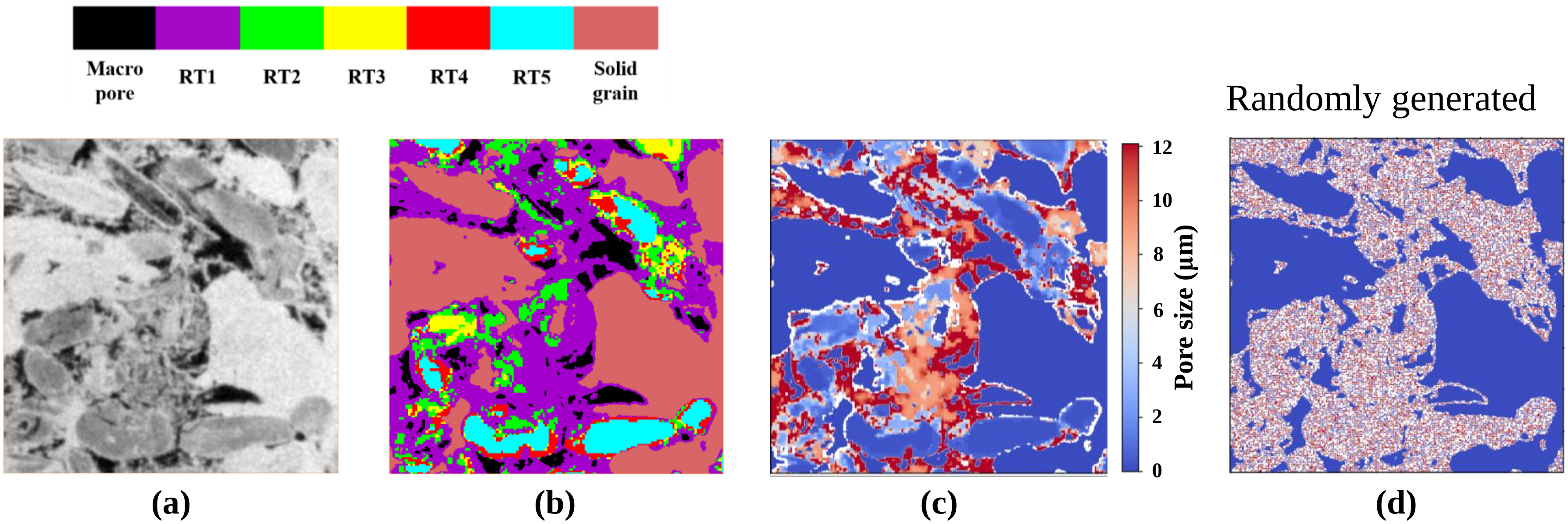
Estimation of microporosity permeability distribution





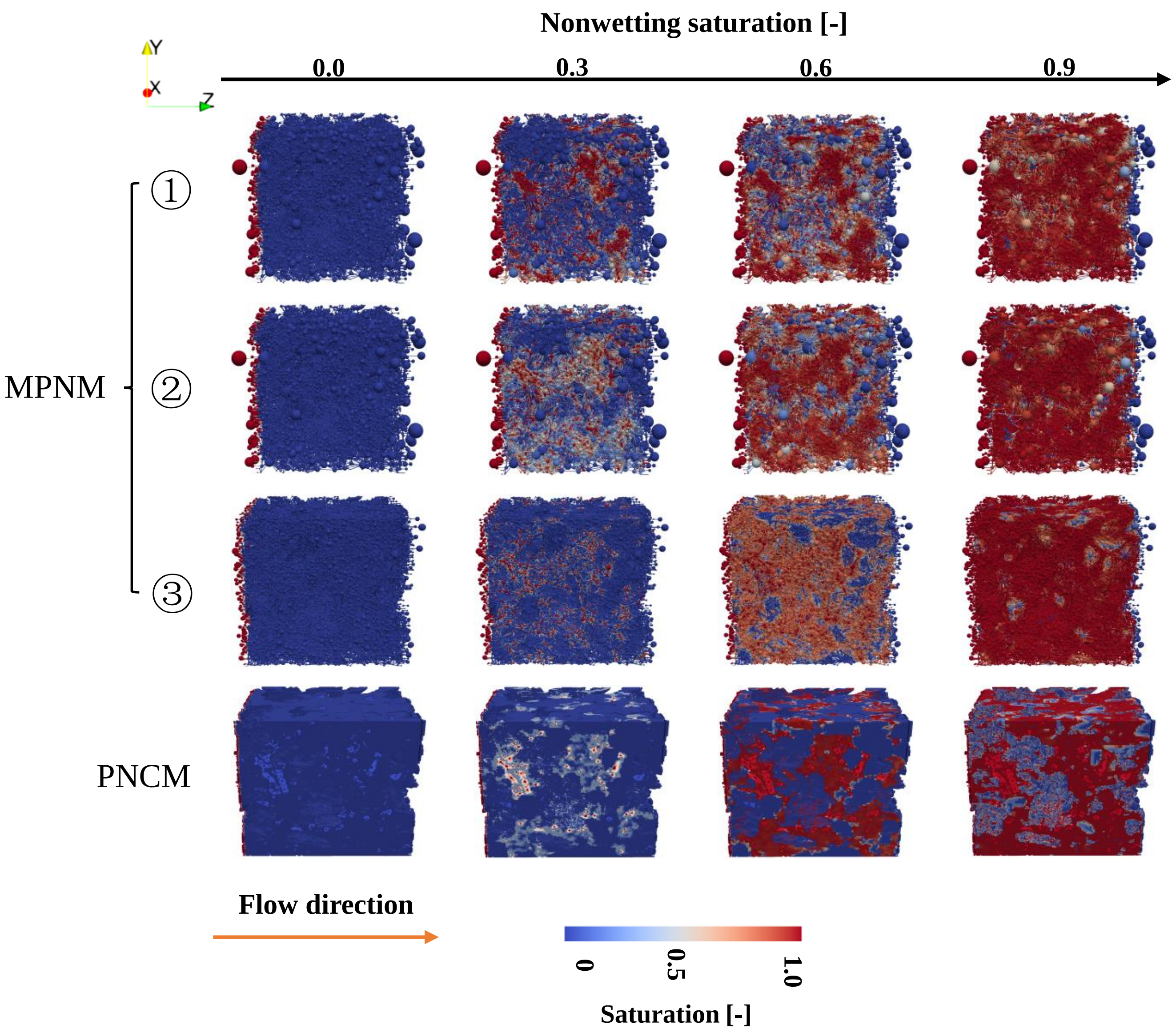


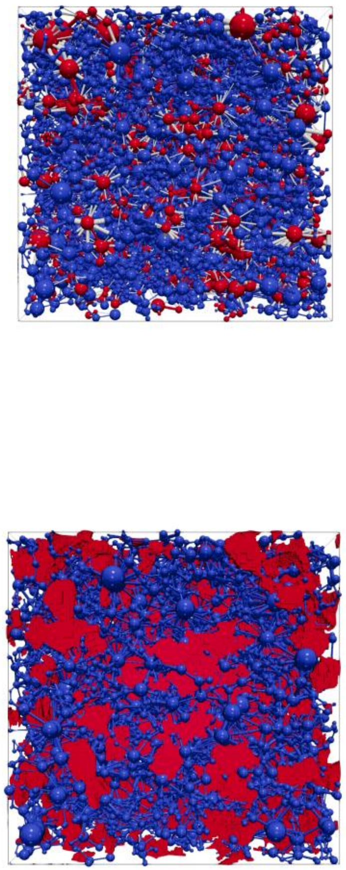
Why do we need the sub-rock typing?



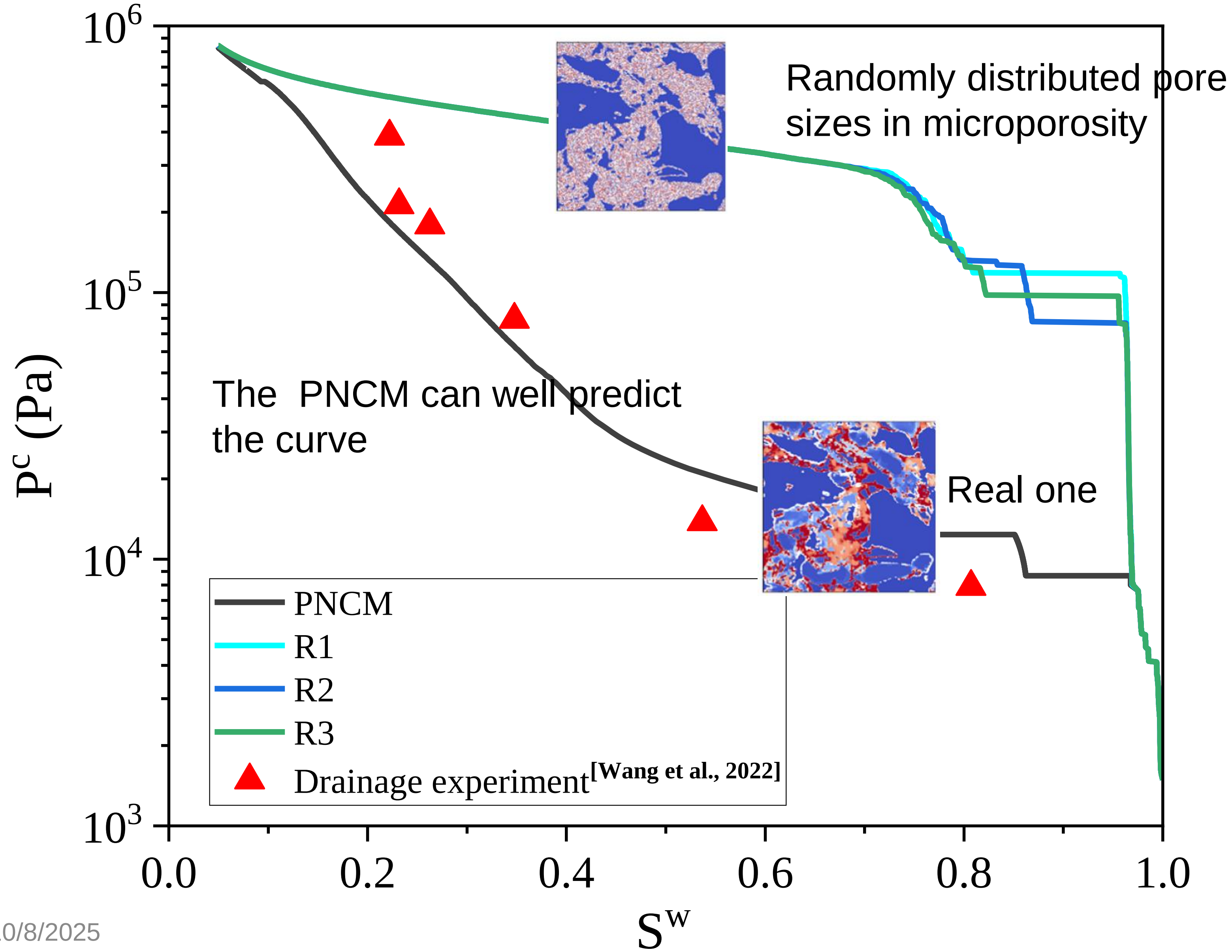
- The sub-rock typing helps with the prediction, but the CT-based characterization is costly and time-consuming !
- If only the MICP data is used, the correlation of pore sizes should be taken into account.

Review the model setup (400^3 sub-volume of ES6.5)

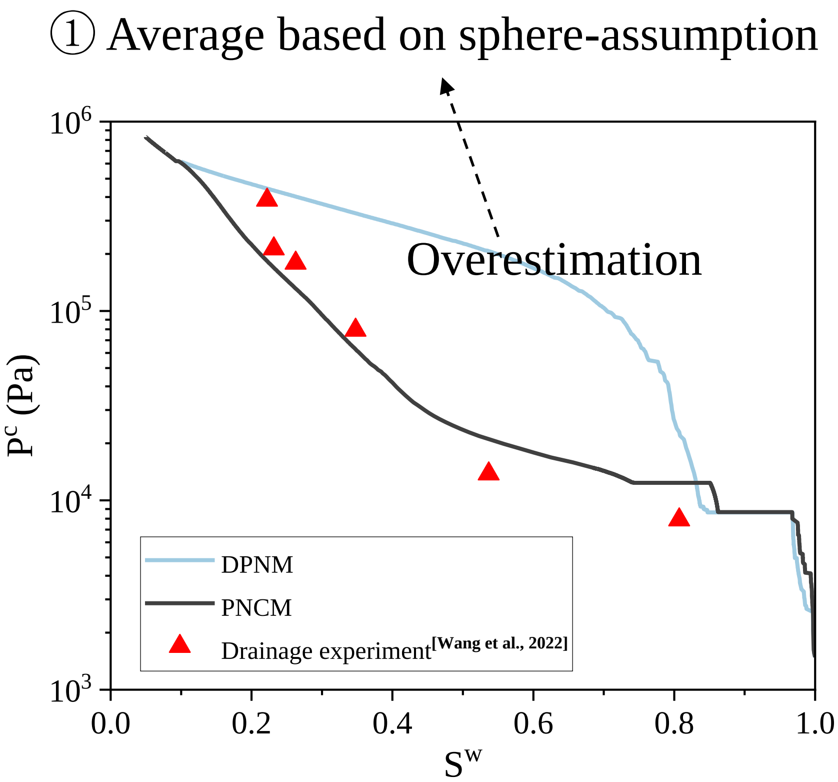


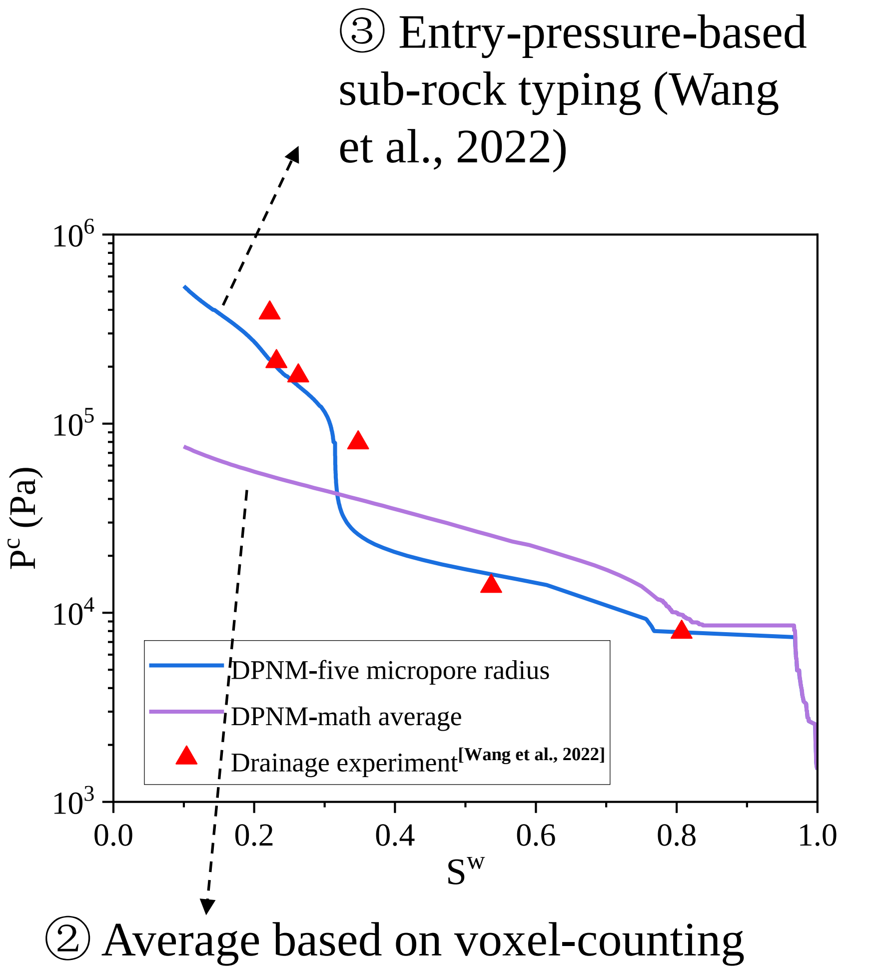


Capillary pressure curve predicted by the PNCM



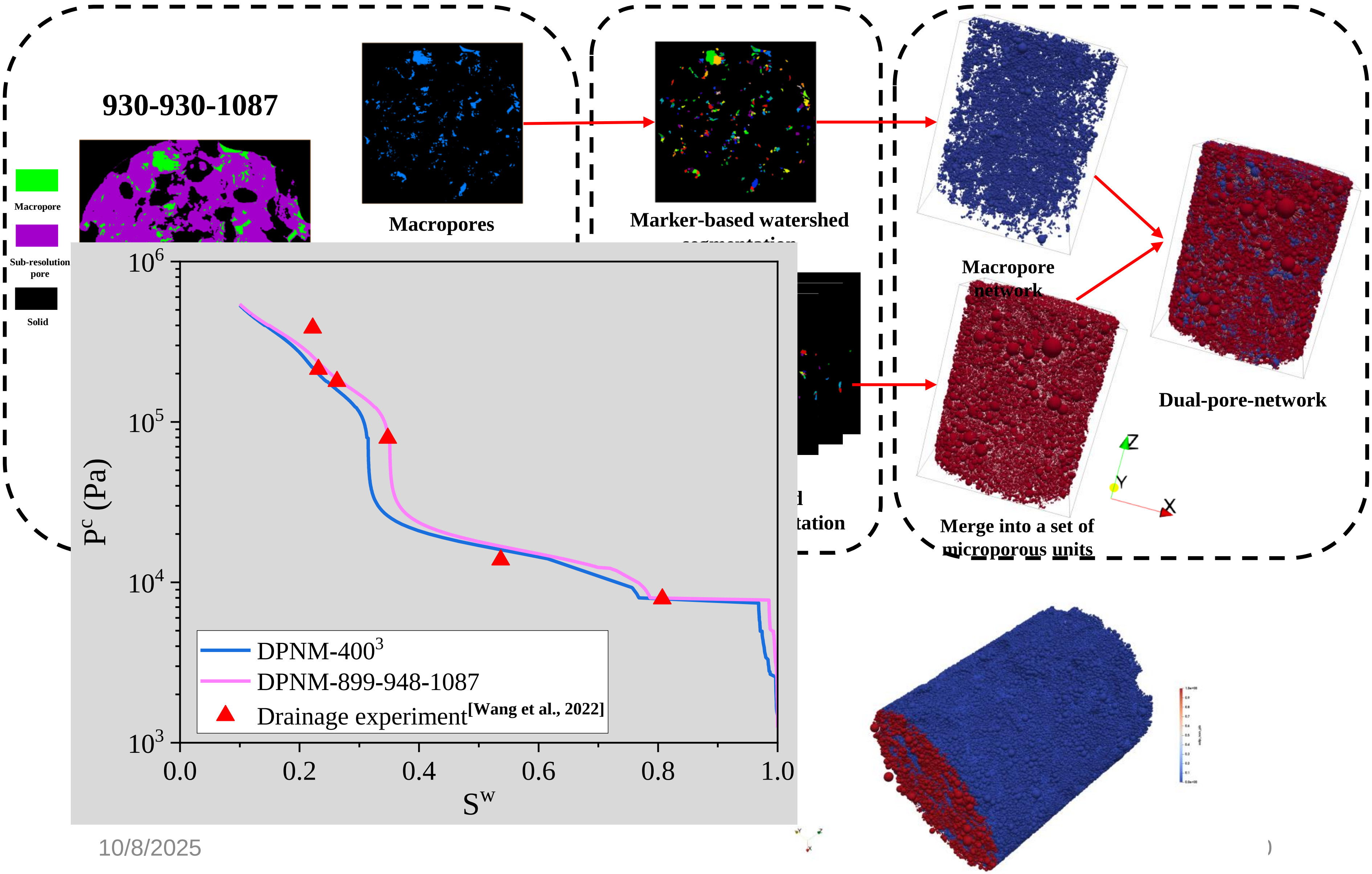
Capillary pressure curve by the MPNM



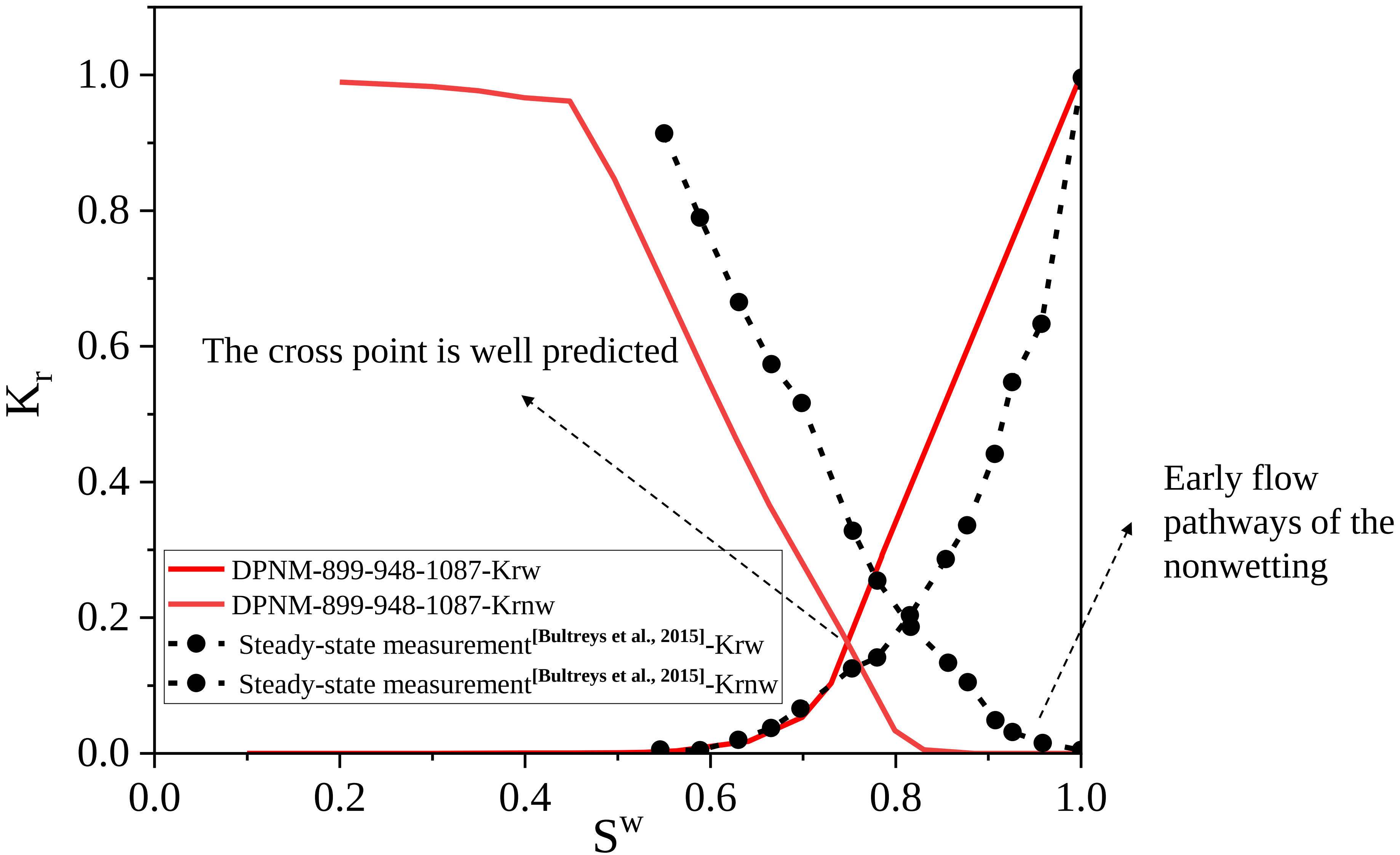


- ❑ The **sub-rock typing** is essential to the efficient multiscale pore-network model.
- ❑ 400^3 size **is adequate to** the prediction of capillary pressure curve.

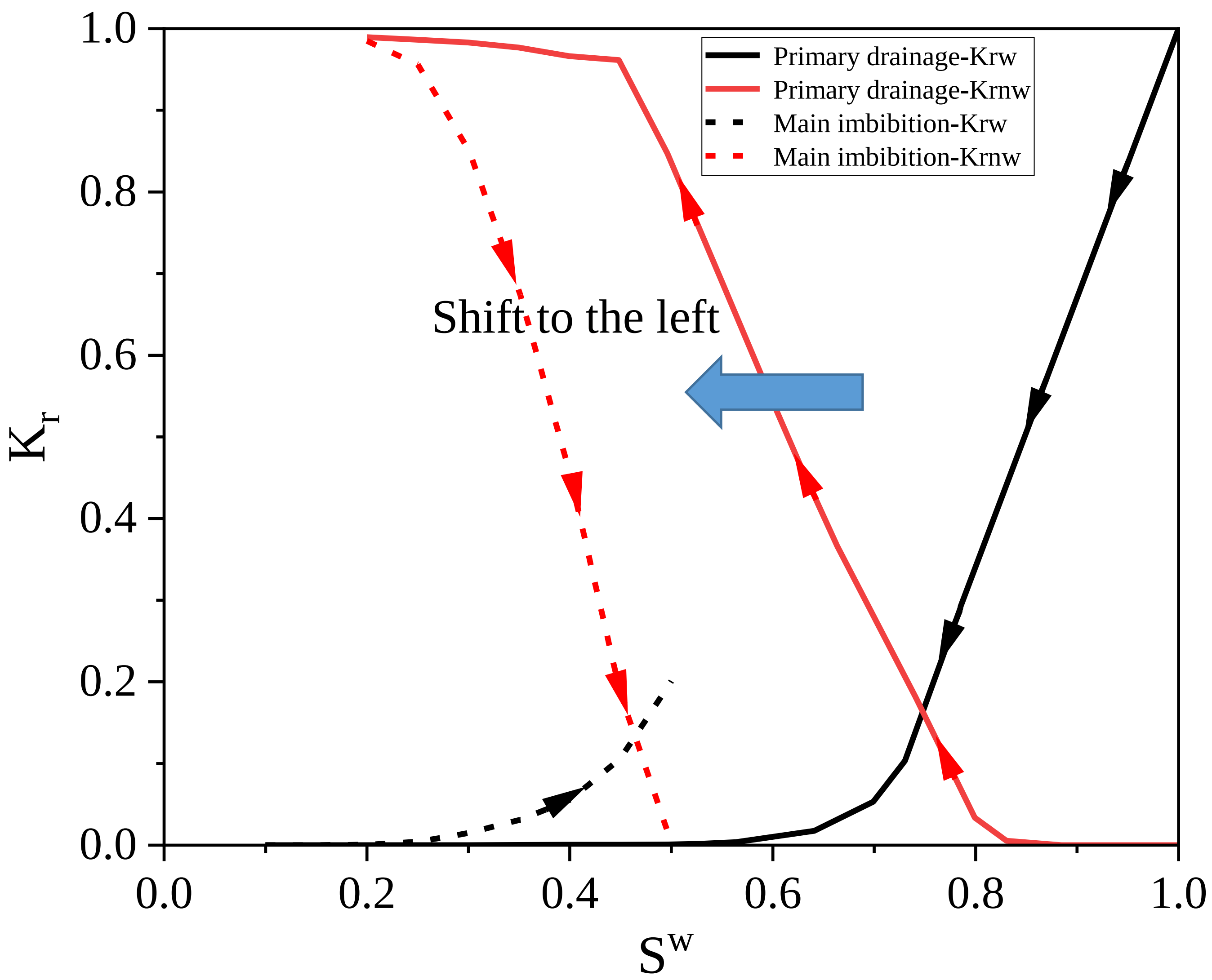
Capillary pressure (the full image of ES6.5)



Relative permeability (the full image of ES6.5)



Relative permeability (the full image of ES6.5)



Outline

1. Introduction of multiscale pore-network model
2. Predictions of absolute permeability and formation factor
3. Predictions of capillary pressure and relative permeability
4. Conclusions and outlook

Conclusions and outlook

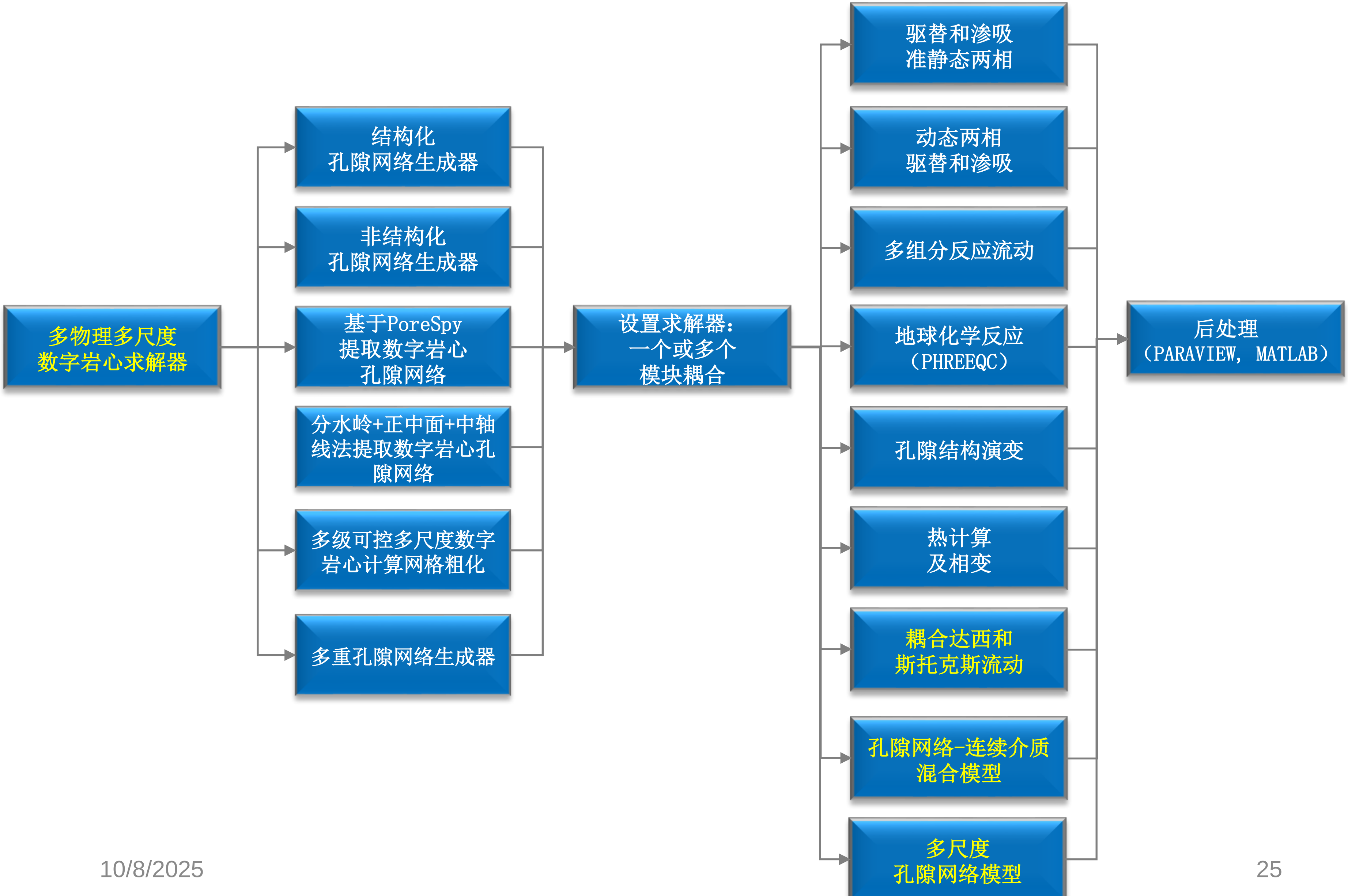
Conclusions

- A high-efficient multiscale pore-network model (MPNM) is developed, and verified against the high-resolution pore-network-continuum model (PNCM).
- Microporosity of ES rocks has strong heterogeneity of mean pore sizes.
- Three types of averaging microporosity voxels are tested. It is found that the sub-rock typing is necessary to guarantee the reliable predictions of both single-phase and two-phase flow parameters.
- We can well predict absolute permeability, formation factor, capillary pressure and relative permeability.

Outlook

- Advance the modeling framework to two-phase flow dynamics.
- Understand how microporosity influences material properties, and extend capillary pressure and relative permeability empirical models.
- Seek for more applications and collaborations.

Multiphysics Multiscale Digital Rock Simulator (MMDRS)



References

1. X. Zhao, B. Shi, X. Wang, J. Zhao, F. Jiang, C.Z. Qin. Modeling of permeability and formation factor of carbonate digital rocks: dual-pore-network and pore-network-continuum models. ***Transport in Porous Media***, 152:37, 2025

2. B. Shi, H. Jiang, B. Guo, J. Tian, and C.Z. Qin. Modeling of flow and transport in multiscale digital rocks aided by grid coarsening of microporous domains. ***Journal of Hydrology***, 633: 131003, 2024.

3. C.Z. Qin, H. van Brummelen, M. Hefny, and J. Zhao. Image-based modeling of spontaneous imbibition in porous media by a dynamic pore network model. ***Advances in Water Resources***, 152: 103932, 2021.

4. L. Zhang, B. Guo, C.Z, Qin, Y. Xiong. A hybrid pore-network-continuum modeling framework for flow and transport in 3D digital images of porous media. ***Advances in Water Resources***, 190: 104753, 2024.

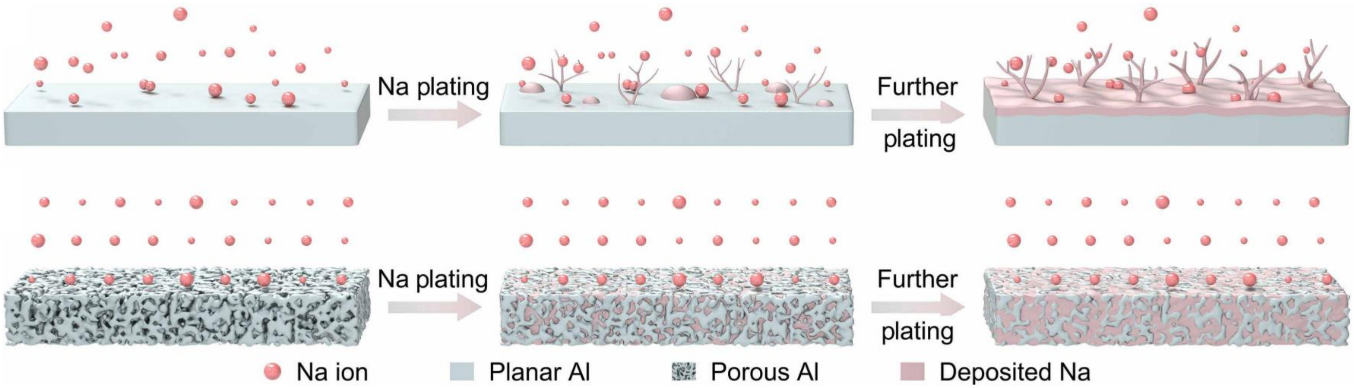
5. H. Jiang, C. Arns, Y. Yuan, C.Z. Qin. SVM-based fast 3D pore-scale rock-typing and permeability upscaling for complex rocks using Minkowski functionals. ***Advances in Water Resources***, 183: 104605, 2024.

6. C.Z. Qin, X. Wang, M. Hefny, J. Zhao, S. Chen, and B. Guo. Wetting dynamics of spontaneous imbibition in porous media: from pore scale to Darcy scale. ***Geophysical Research Letters***, 49, e2021GL097269, 2022.

Thank you for your attention!

Research challenges for flow and transport

Reduce Na dendrites



Design of porous anode current collectors

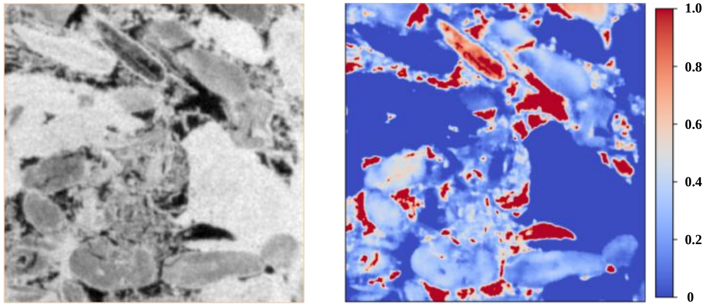
Test samples of carbonate digital rocks

https://www.digitalrocksportal.org/

Digital rock	Voxel size (μm)	Microporosity	Image size (voxels)	Total Porosity (%)	Absolute permeability (mD)
					Experimental
ES3.1	3.1	Uniform mean pore size	2000×2000×1725	25	260 ± 60
ES3.6	3.6	Uniform mean pore size	1000×1000×1000	29	/
ES6.5	6.5	Heterogeneous	1316×1316×1087	25	202.4 ± 86.9

ES3.1 and ES3.6 have the MICP curves; ES6.5 has **the porosity map and the entry-pressure map** of subresolution microporosity.

The porosity map of ES6.5



(a) (b)

Predictions of absolute permeability and formation factor

Subvolume of digital rock	Pore regions	Original voxels	Volume fraction	In the MPNM	In the PNCM
ES3.1	Macropores	6332318	9.9%	3569	3569
	Microporosity	21562493	33.7%	8375	3929815
ES3.6	Macropores	5040267	7.9%	2172	2172
	Microporosity	32676964	51.1%	13228	4494989
ES6.5	Macropores	3694907	5.8%	3827	3827
	Microporosity	40618405	63.5%	7930	4147069

90% reduction in computational grids

Why does the MPNM underestimate the absolute permeability?

Digital rock	Mean pore size (μm)	By the MPNM (mD)	By the PNCM (mD)	By the reference model (mD)
ES3.1	0.61	109	116	117
ES3.6	0.74	34	37	37
ES6.5-1	1.81	28	18	18
ES6.5-2	Estimated by entry pressure	12	128	174

Digital rock	By the multiscale pore-network model (-)	By the pore-network-continuum model (-)	By the reference model (-)
ES3.1	17.24	19.61	19.23
ES3.6	23.81	23.81	23.26
ES6.5	18.52	20.41	19.23

The prediction of formation factor is satisfied