

# Digital twins

## Synthetic and real porous materials

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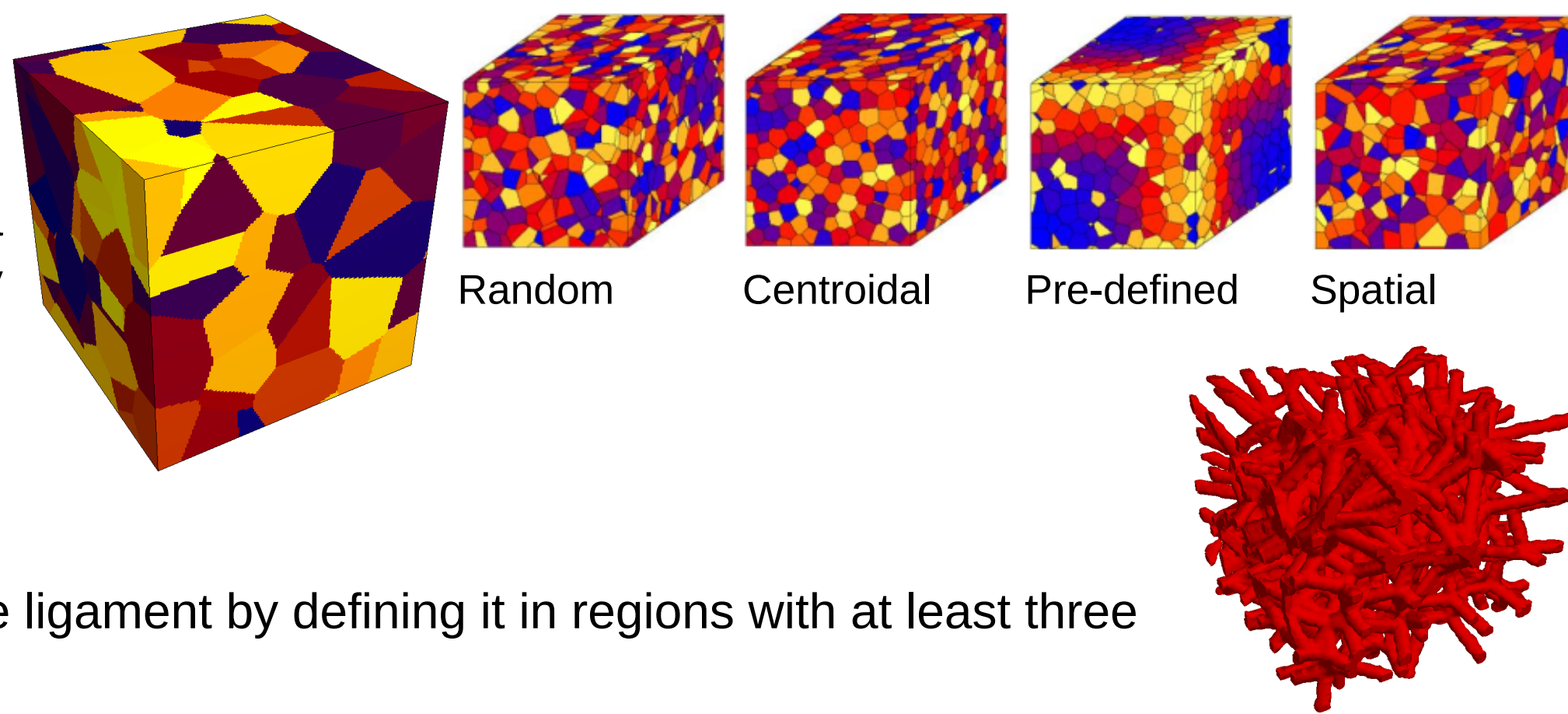
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### Synthetic metal foams: Computer-aided design

Due to their intricate pore network, synthetic metal foams have unique properties that make them attractive for a variety of applications. For instance, lightweight structures benefit from larger pores and thinner ligaments, maximizing porosity while maintaining structural integrity. Conversely, load-bearing structures can be designed with smaller pores and thicker ligaments to enhance mechanical performance. Therefore, designing metal foams for optimal performance requires precise control over their internal structure. Computer-aided design (CAD) is proving to be a powerful tool in this regard. By allowing manipulation of pore size and ligament morphology, CAD facilitates the creation of foams with tailored properties. Understanding the impact of CAD on the behavior of these foams under various conditions remains an active area of research. Ultimately, CAD empowers scientists and engineers to unlock the full potential of synthetic metal foams. By manipulating pore arrangements and ligament designs, these materials can be tailored for specific applications, driving advances in fields such as energy and infrastructure development.

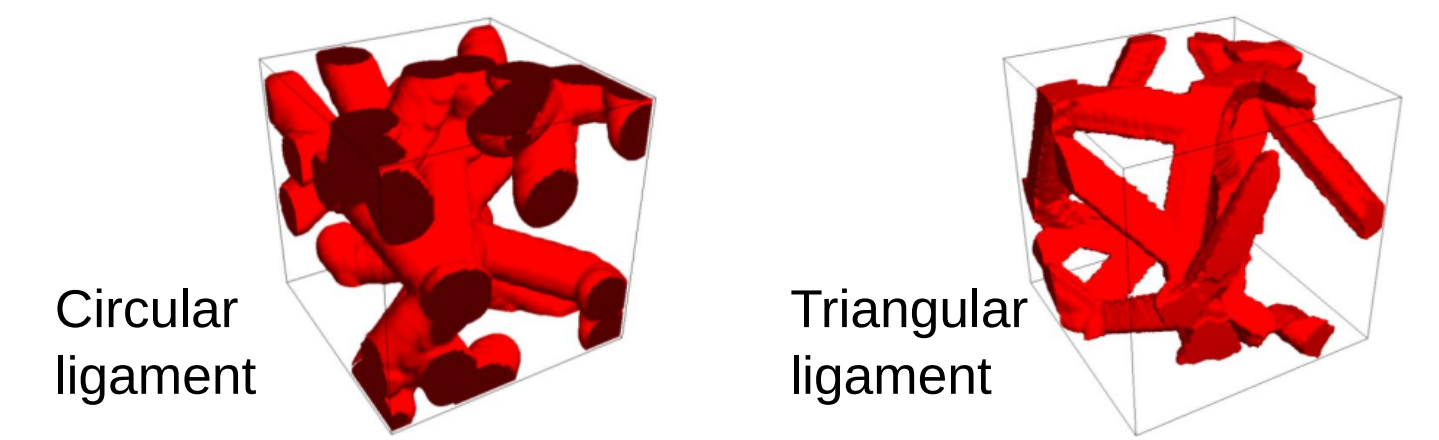
#### Pore distribution

Dictate how pores are arranged within the material, such as Voronoi tessellation, which creates a network of interconnected pores by dividing space into regions based on proximity to "seed points".



#### Fine-tuning functionality

- Pore and ligament dimensions: Control the size of the pores and the solid ligaments.
- Total pore count: Define the exact number of pores in the structure.
- Porosity: Manipulate the total void volume within the material.
- Ligament morphology: Precisely design the cross-sectional shape (e.g., circular, triangular) and thickness of ligaments for specific mechanical properties.



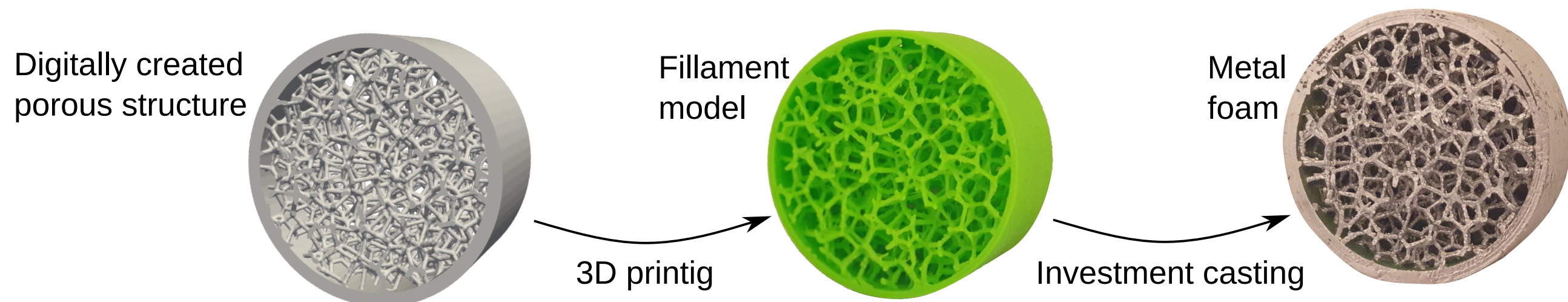
#### Ligament Design

Specify the desired properties of the ligament by defining it in regions with at least three adjacent (Voronoi) cells.

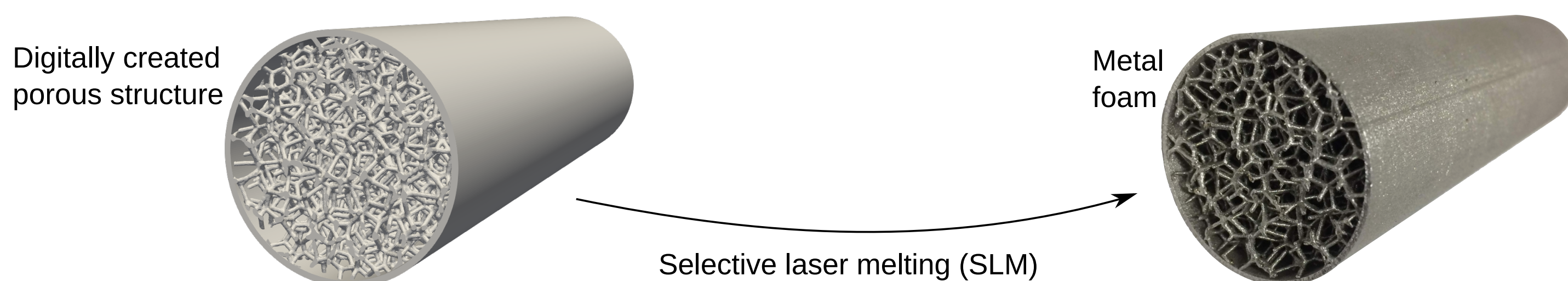
### Digital-to-real translation

#### Fabrication of metal foams using additive manufacturing

■ A synthetic porous structure, represented as a three-dimensional (3D) digital model, is translated into a file suitable for 3D printing. This file is then fabricated using an extrusion-based 3D printer. The resulting 3D-printed model is subsequently invested with a ceramic mold material. Through investment casting, a metallic replica of the original synthetic design is achieved.



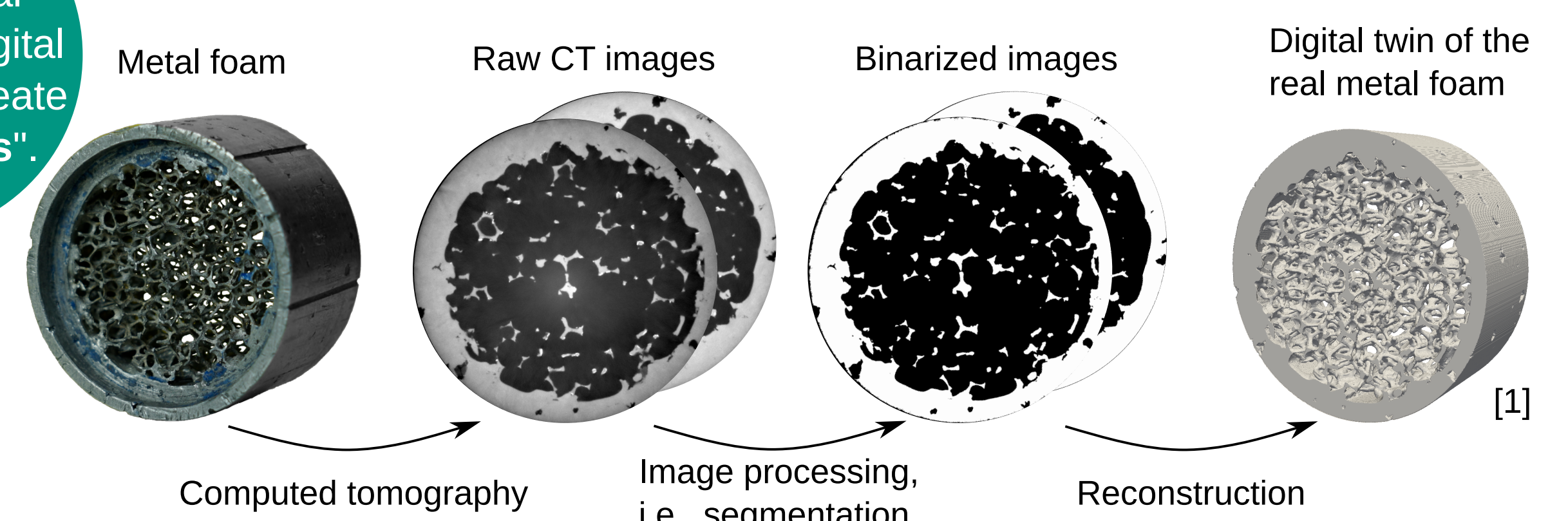
■ The computer-generated porous structure can be directly manufactured as a metal foam using laser-based metal additive manufacturing (selective laser melting, SLM).



### Real-to-digital translation

#### Digital twins of real porous structures

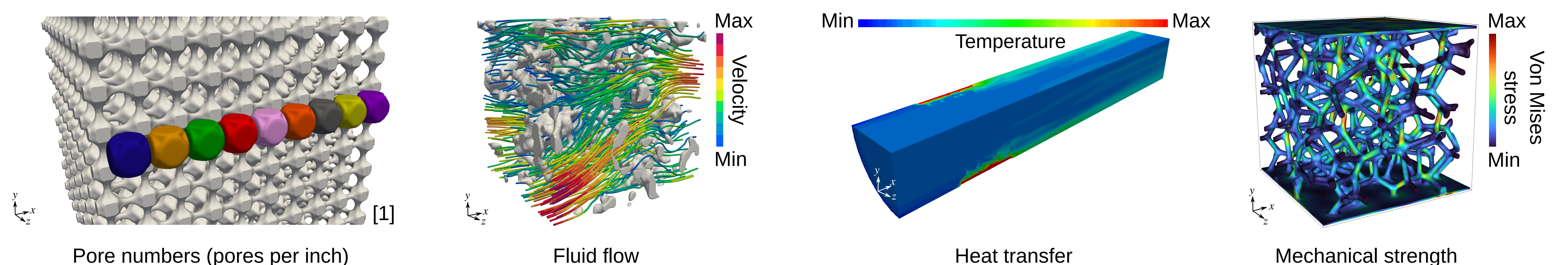
The intricate internal structure of open-cell metal foams can be identified using imaging techniques such as computed tomography (CT), which produces a series of grayscale images. Image processing techniques are then used to distinguish between the solid and void spaces. This process, known as segmentation, involves applying a threshold to the grayscale data, which is converted to a binary format. After segmentation, the stack of binary images is reconstructed. This process transforms the two-dimensional image data into a 3D representation of the porous structure.



Both Digital-to-real and real-to-digital translations create "digital twins".

### Numerical investigations

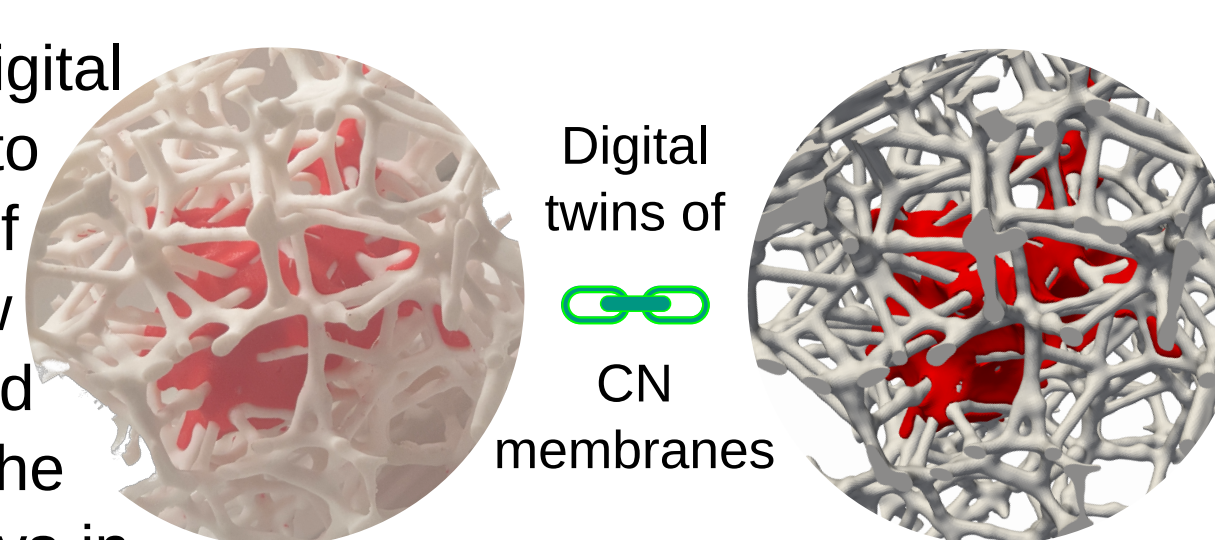
A digital representation of the porous structure allows for a variety of computational analyses. Morphological characterization, including quantification of pore size distribution and number, can be performed. Simulations of physical phenomena are also possible, including modeling of fluid flow, heat transfer, and mechanical behavior of the porous material.



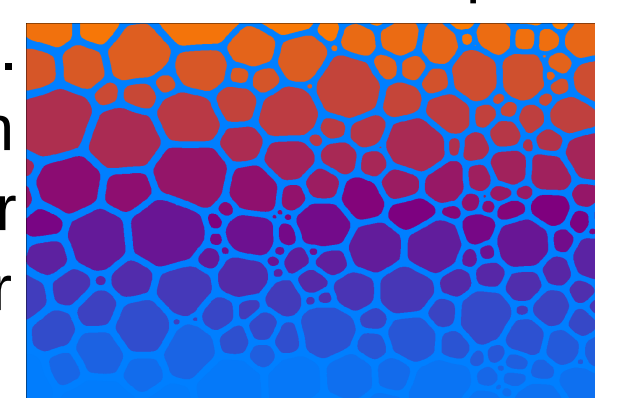
### Digital porous structures: Data-driven design

The development of digital representations of various porous materials has become a powerful tool for data-driven design and optimization in various scientific fields. Two prominent examples illustrate this impact.

■ Cellulose nitrate (CN) membranes: Digital models of CN membranes are used to optimize lateral flow assays. Simulations of fluid flow within the membrane pores allow researchers to refine pore size and distribution, ultimately improving the sensitivity and specificity of these assays in detecting target molecules.



■ Liquid polymer foams: Digital models of liquid polymer foams are used in the design and development of metal foams. This data-driven approach facilitates the tailoring of the final metal foam pore morphology (size, distribution, interconnectivity). This enables the creation of metal foams with desired properties, such as high porosity for lightweight applications or specific pore sizes for filtration purposes.



[1] Jamshidi et al., A 3D computational method for determination of pores per inch (PPI) of porous structures, Materials Today Communications, vol. 34, p. 105413, 2023.