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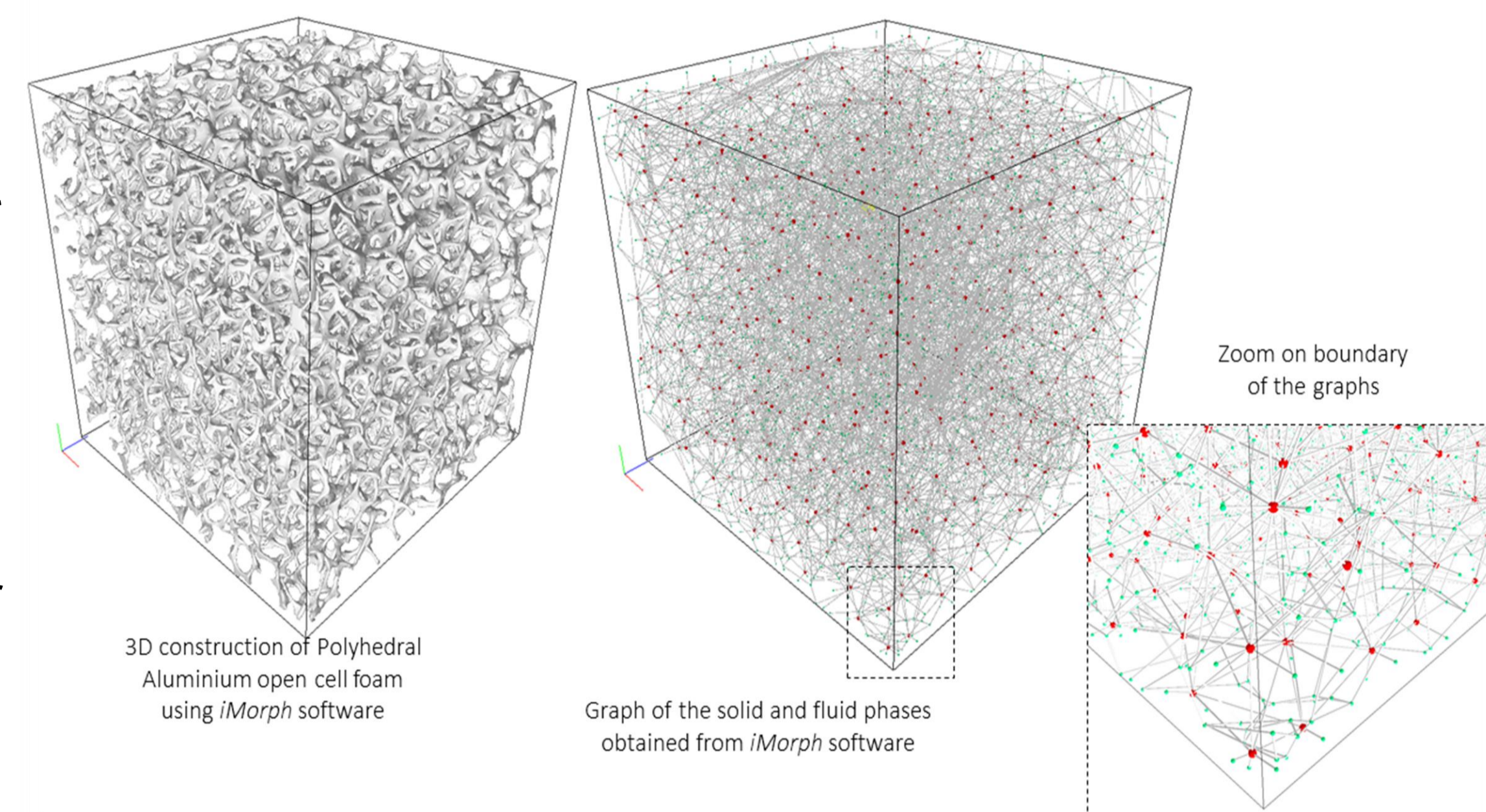
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Motivation

Open metal cell foams have a number of particular properties, such as lightness, mechanical resistance, thermal properties, energy absorption, which are of a great interest in different applications such as structured catalytic reactors (*Banhart, 2001; Bianchi et al., 2012*).

→ An accurate model of heat and mass transfer is needed for process control and design. Homogeneous models fail to accurately represent the anisotropic and irregular structure of foams and the CFD modelling requires high computationally expensive discretization.

→ We are interested in structured modelling of mass and heat transfer in two phases, determined by the topology of the foam and generate low computational cost simulation.



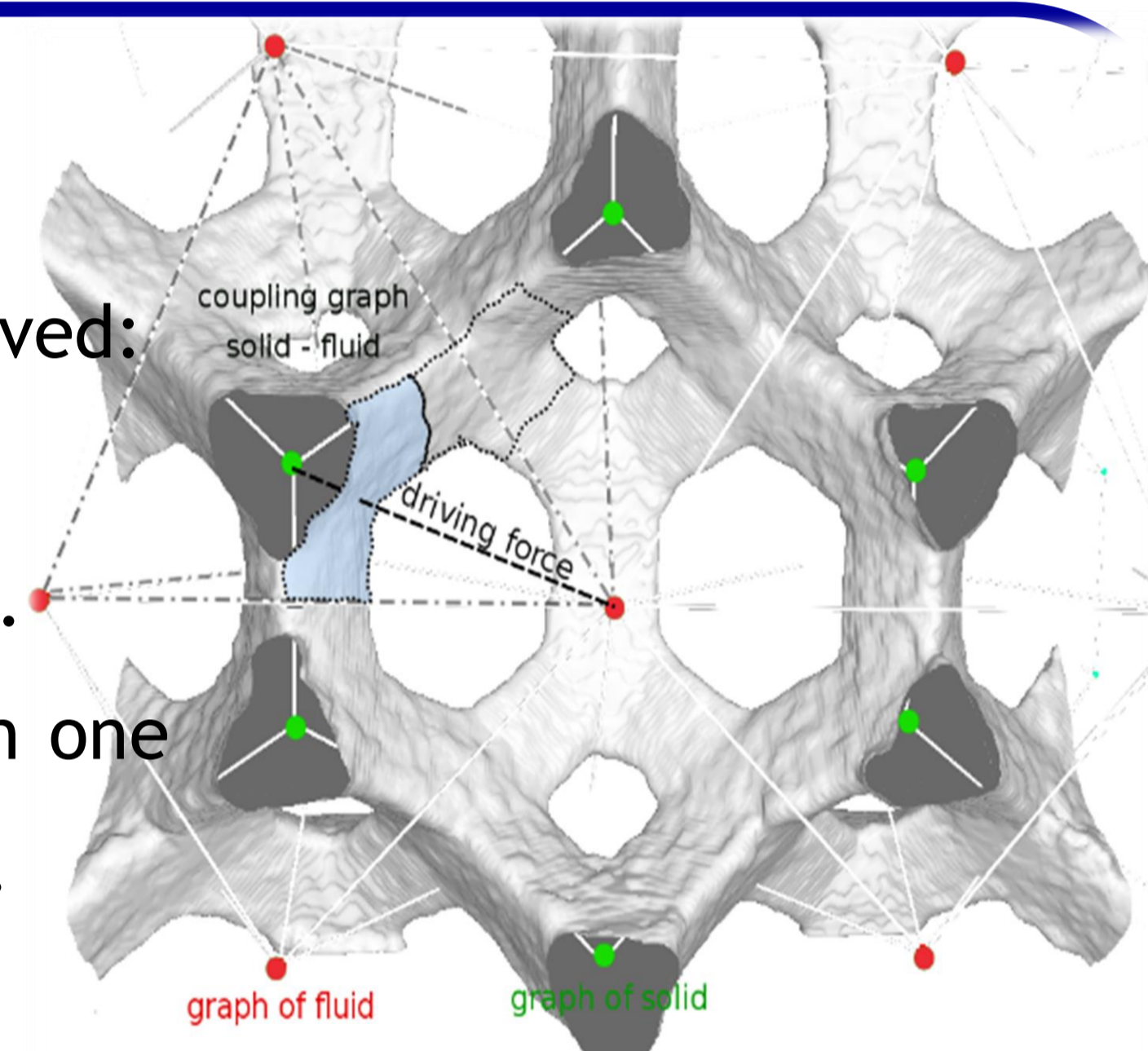
Construction of the solid and fluid graphs using x-ray CT and iMorph

Methodology

1. Graph construction : from x-ray CT images and using iMorph© software (*Brun et al., 2008*), graphs are derived:

- The **graph of solid**, one associates nodes to adjacent half-struts and edges to interfaces.
- The **graph of fluid**, one associates nodes to pores volumes and edges to surfaces at the interface of two pores.
- The **coupling graph** is used to account for interphases transfer phenomena. A driving force is defined within one node of solid and one node of fluid and heat fluxes within the surface of solid nodes (See Figure on the right).

Geometrical properties (e.g. node volume), are extracted and associated with the elements of the graph.



2. Construction of K-complexes

The K-complex is a set of discrete objects of various dimensions (*Poincaré, 1895; Tonti, 1976*).

Physical Variables	Geometrical Objects
Energy U_i	Node / pore volume v_i
Heat flux ϕ_i	Faces / Interfaces f_i
Driving force F_{ij}	Edges e_i
Temperature T_i	Nodes n_i

3. Conservation laws on K-complexes : Port-Hamiltonian Systems (*Kotyczka & Maschke, 2017*)

Heat equation for a thermal conductivity λ

$$\rho C \frac{\partial}{\partial t} T(x, t) = -\text{div } \phi$$

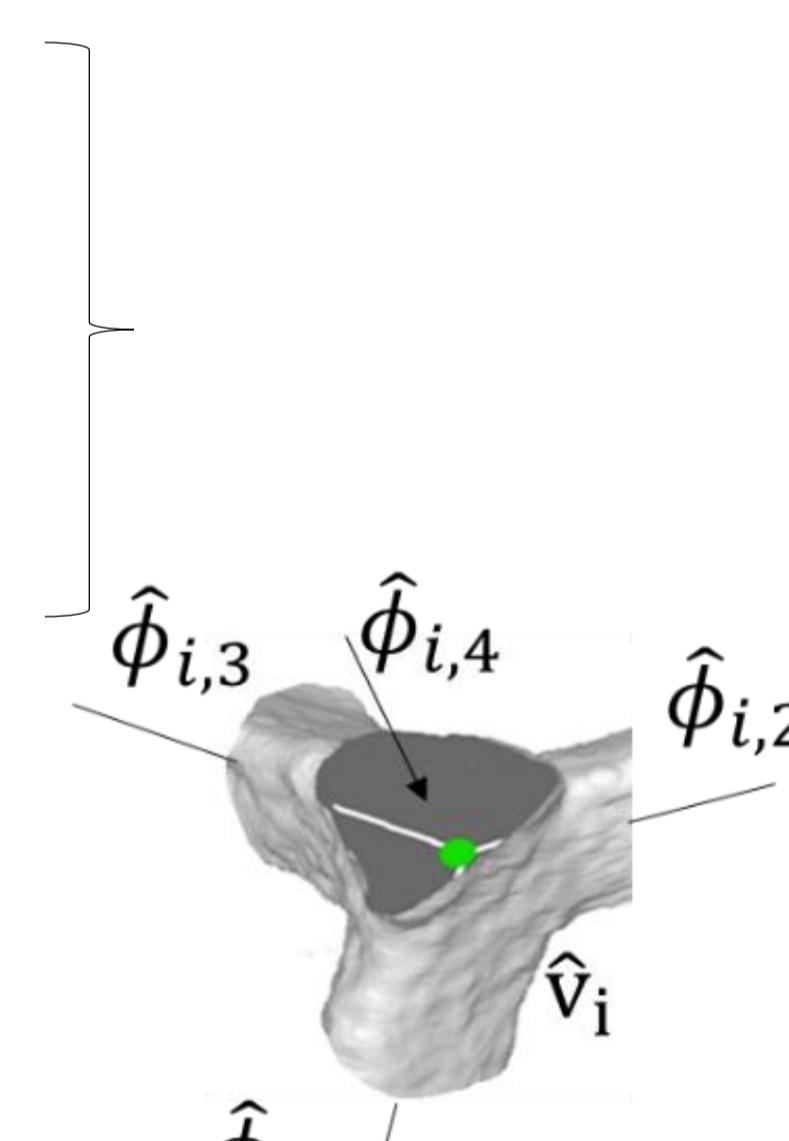
Heat flux obeys Fourier's law

$$\phi = -\lambda F_{ij} \quad , F_{ij} = T_j - T_i$$

Discrete balance equation on v_i

$$\frac{d}{dt} \int_{v_i} u_i dv = - \int_{\partial v_{ij}} \phi_{ij} ds$$

where D is the co-incidence matrices constructed from the topology of the foam. Index b for boundary.



$$\begin{bmatrix} \frac{\partial}{\partial t} U(x,t) \\ F(x,t) \end{bmatrix} = \begin{bmatrix} 0 & -\text{div} \\ -\text{grad} & 0 \end{bmatrix} \begin{bmatrix} T(x,t) \\ \phi(x,t) \end{bmatrix}$$

Extensives variables Interconnection matrices Intensives variables

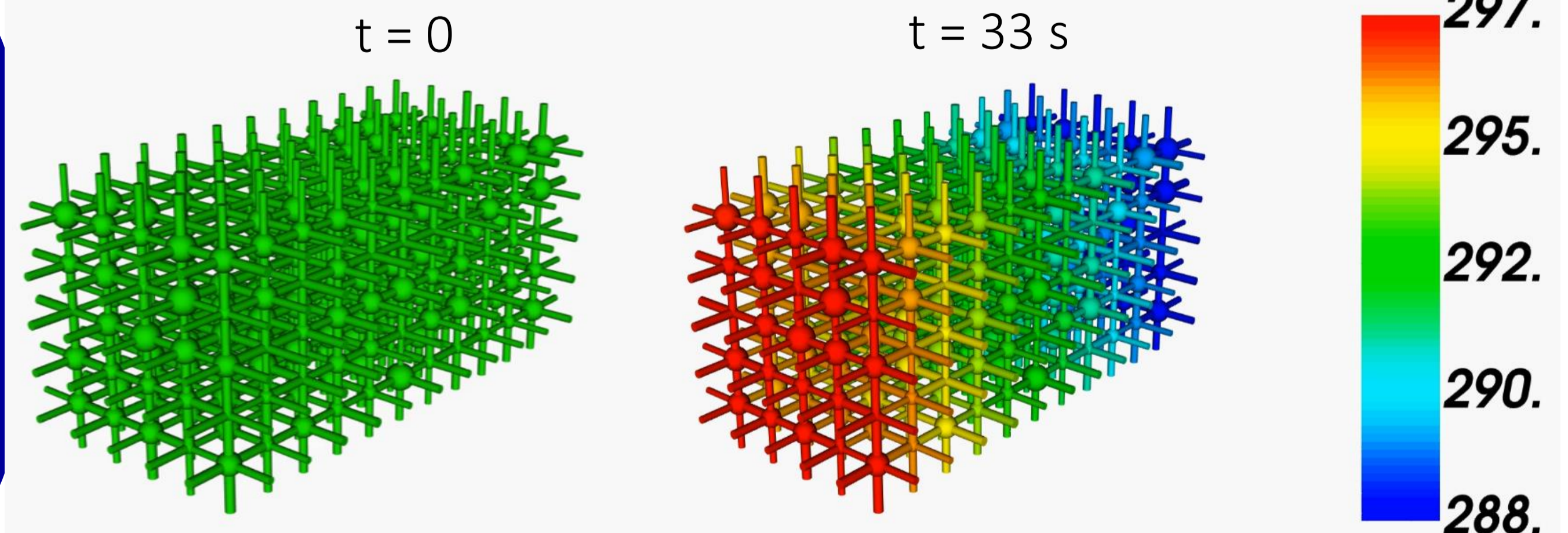
Finite-dimensional Port Hamiltonian Systems

$$\begin{bmatrix} \frac{\partial u_i}{\partial t} \\ F_{ij} \end{bmatrix} = \begin{bmatrix} 0 & D \\ -D^T & 0 \end{bmatrix} \begin{bmatrix} T_i \\ \phi_{ij} \end{bmatrix} + \begin{bmatrix} D_b \\ 0 \end{bmatrix} \phi_b$$

Results

A numerical virtual open cell foam with regular structure and different node sizes was constructed and used as an example for simulating heat transfer. The foam initially at a temperature $T = 292$ K, is heated from the left side and cooled from the right side.

This simulation was performed using Python™ and was observed for 30s real time. The gain in the computational time is clearly achieved.



Conclusions

The methodology of the graph based approach using port Hamiltonian Systems is presented. Starting from x-ray CT scans, the 3D numerical foam is constructed using iMorph → Graphs are constructed based on topological and geometrical description and defined with respect to physical phenomena → The K-complexes are constructed based on the graphs and physical variables are attributed to discrete objects → The discrete balance equations are then evaluated on K-complexes as PHS.

Future works

- Modelling of real structure open cell foams with large size.
- Comparison with experimental measurements for validation
- model reduction while preserving the interconnection interfaces and the original PH structure.

