Numerical Approximation of Heat Transfer on Heterogenous Media

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In this paper we show the discrete modeling of the heat equation on an open cell metallic foam, exploiting its geometric structure. The topology of the material is described using the incidence matrices of a so called k-complex. Together with the discrete constitutive equations, a finite-dimensional model in port-Hamiltonian form is found.

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1 Introduction

In this paper we provide an approach to model heat transfer on open cell foams as shown in Figure 1. These foams are commonly used in industrial applications, e.g. as catalysts for the production of hydrogen [1]. A numerical model of the heat transfer on the foam is needed for design optimization and control of the chemical process. Figure 2 shows an experimental setup to determine the macroscopic properties of the foam. A tomography picture of an open cell foam from which the graph structure can be extracted via image processing¹ is shown in Figure 3.

Fig. 1: Open cell foam
Fig. 2: Experiment
Fig. 3: Tomography data

For numerical simulations, models with different levels of detail can be found in the literature. A rather coarse approach is to approximate the behavior of the entire block of foam by surrogate parameters [3]. In contrast to this approach, standard finite elements can be used on a very fine mesh [4]. In between these extrema, the resistive approach [5] can be found, which approximates the heat transfer by a network of thermal resistances.

In the presented approach, we evaluate the heat equation on the topological objects defined by the material structure and model the heat exchange between the corresponding objects on the material and the fluid phase, respectively. Our goal is to obtain a port-Hamiltonian (PH) model which can be easily coupled with other subsystems and augmented by additional physical effects like convection. PH systems consist of storage and dissipation elements connected by a power preserving Dirac structure. The power flowing into each element is described by the product of conjugated port variables, so called flows and efforts. Ports can also be defined w.r.t. other exchanged quantities, e.g. an entropy flux. For an introduction to PH systems and the power based modeling of multiphysics systems see [6].

2 Cell Method and Construction of Dual k-Complexes

The heat transfer in the open cell foam is described using the cell method [7, 8], which we want to briefly introduce. In this paper we restrict ourselves for illustration purposes to the case of cubic foams with their particularly simple structure.

2.1 Geometric Objects: j-Cells

The physical variables to describe heat transfer are connected to geometric objects, called j-cells, where j denotes the spatial dimension of the geometric object. In 3D, there are nodes (0-cells), edges (1-cells), faces (2-cells) and volumes (3-cells). All j-cells have an inner and an outer orientation, as shown in Figures 4 and 5. A k-complex is a sequence of spaces of j-chains (formal sum of j-cells), connected via the boundary map ∂j with the property ∂j−1 ∘ ∂j = 0 for j = 2, ..., k [9].

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¹ http://imorph.sourceforge.net, developed by Emmanuel Brun and Jérôme Vicente

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2.2 $k$-Complex and Its Dual

The topology of a $k$-complex can be described using incidence matrices (the matrix representations of the boundary maps $\partial_j$) that contain the numbers $-1$, $0$ and $1$, according to the orientation of the cells. For a given complex as shown in Figure 6, a dual complex is defined by construction. The rough outline of the construction is given in the following, for more details see [10]. The boundary needs special care, depending on the imposed boundary conditions [11].

1. Dual nodes are located inside each primal volume.
2. The dual nodes are connected by dual edges that cross the primal faces.
3. A dual face is constructed around each primal edge.
4. Dual volumes are defined such that each dual volume has one primal node inside.

Figure 7 shows the dual 3-cell around an interior node of the primal complex, we also omit the arrows which indicate the orientation of each $j$-cell.

3 Discrete Heat Equation on One Phase

To obtain a discrete description of the heat transfer, we start with the continuous case and reshape the equations so that they can be discretized in a structured way. The well known heat equation with constant coefficients can be written as a second order partial differential equation (PDE) on $\Omega \subset \mathbb{R}^k$ with boundary $\partial \Omega = \partial \Omega_D \cup \partial \Omega_N$

$$c \frac{\partial}{\partial t} T(x,t) = \lambda \Delta T(x,t)$$  \(1\)

with temperature $T$, heat capacity $c$ and thermal conductivity $\lambda$. $T(x,0) = T_0(x)$ denotes the initial condition and

$$T(x,t) = u_D(x,t), \quad x \in \partial \Omega_D$$

$$\nabla T(x,t) \cdot n(x) = u_N(x,t), \quad x \in \partial \Omega_N$$  \(2\)

are imposed boundary conditions (inputs).

We rewrite this equation as a first order PDE system

$$\begin{bmatrix} -\frac{\partial}{\partial t} U(x,t) \\ F(x,t) \end{bmatrix} = \begin{bmatrix} 0 & \text{div} \\ \text{grad} & 0 \end{bmatrix} \begin{bmatrix} T(x,t) \\ Q(x,t) \end{bmatrix}, \quad U = cT, \quad Q = -\lambda F$$  \(3\)

with the internal energy density $U$, the heat flux density $Q$, the thermodynamic driving force $F$ and the constitutive laws. In the language of PH systems, the formally skew-adjoint differential operator separates the flow variables on the left hand side from their conjugate counterparts, the efforts, on the right hand side. Equation (3) can be written in an elegant way by using differential forms [12]

$$\begin{bmatrix} -\frac{\partial}{\partial t} U \\ F \end{bmatrix} = \begin{bmatrix} 0 & (-1)^{k-1} \text{d} \\ \text{d} & 0 \end{bmatrix} \begin{bmatrix} T \\ Q \end{bmatrix}, \quad U = c \ast T, \quad Q = (-1)^k \lambda \ast F$$  \(4\)
with \( U \in \bigwedge^k(\Omega) \), \( T \in \bigwedge^0(\Omega) \), \( F \in \bigwedge^1(\Omega) \) and \( U \in \bigwedge^{k-1}(\Omega) \) differential forms of corresponding degree. \( d : \bigwedge^j(\Omega) \to \bigwedge^{j+1}(\Omega) \) is the exterior derivative as a unified differential operator. The Hodge star \( * \) transforms a \( j \)-form to a \( (k - j) \)-form [13]. Integral variables (like the total energy on a \( k \)-cell) are evaluated on their appropriate geometric objects on the primal and dual complex, as shown in Table 1. In the discrete setting, the operators are replaced by their discrete counterparts [14, 15].

Table 1: Physical variables and integration domains for the PH modeling of heat transfer.

| Physical Variable | Geometric Object | Physical Variable | Geometric Object |
|------------------|-----------------|------------------|-----------------|
| \( \hat{U}_i \)  | Dual volume \( \hat{\eta}_i \) | Temperature \( T_i \) | Primal node \( n_i \) |
| Driving Force \( F_m \) | Primal edge \( \hat{c}_m \) | Heat transfer rate \( \hat{\Phi}_m \) | Dual face \( \hat{f}_m \) |

We now derive the discrete counterpart of Equation (4). The discrete energy balance is found by evaluating the heat flux that goes through the dual faces of a dual volume, as shown in Figure 8.

\[
\frac{\partial}{\partial t} \hat{U}_i = \sum_n \hat{\Phi}_{i,p}
\]

where the index \( i \) denotes the global number of the volume and \( p \) is the local number of its boundary face. The discrete driving force is evaluated on the primal complex

\[
F_m = -\frac{T_{m,1} - T_{m,2}}{||r_{m,1} - r_{m,2}||}.
\]

Here, the index \( m \) denotes the global number of the edge that the driving force is connected to.

Fig. 8: Balance of internal energy

With the use of the co-incidence matrices (which are the transposed incidence matrices) \( \hat{d}_i^k \) and \( \hat{d}_i^0 \) [11, 15], we find the discrete representation of the heat equation

\[
\dot{\hat{U}} = \sum_i \hat{\Phi}_{i,p} - \hat{\Phi}_{i,s}
\]

with \( \dot{T} = \frac{C^{-1} \Phi}{\Lambda} \hat{U} \)

where \( \hat{U} \) and \( F \) are vectors that collect \( U_i \) and \( F_m \) respectively. \( C^{-1} \) and \( \Lambda \) are diagonal matrices with the coefficients \( c_i^{-1} \) and \( \lambda_m \) that follow from the discretization of the constitutive equations.

4 Discrete Heat Equation on Two Phases

To construct the equations for two phases, we evaluate the heat equation for both of them as presented before and couple the two phases via the discrete relation \( \hat{\Phi}_i^{fs} = \alpha_i \hat{F}_i^{fs} \) with heat transfer coefficients \( \alpha_i \) (collected in the diagonal matrix \( \alpha \)). This results in the coupled energy balance (Figure 10).

\[
\frac{\partial}{\partial t} U_i^{s,f} = -\sum_p \hat{\Phi}_{i,p} - \hat{\Phi}_{i,s} \quad \frac{\partial}{\partial t} \hat{U}_i = -\sum_p \hat{\Phi}_{i,p} + \hat{\Phi}_{i,s}
\]

where the upper indices \( s \) and \( f \) denote the solid and fluid phase respectively. The driving force is also calculated for both phases (see Figure 11), as well as the temperature difference between the two phases.

\[
F_m^{s} = -\frac{T_{m,1}^{s} - T_{m,2}^{s}}{||r_{m,1} - r_{m,2}||} \quad F_m^{f} = -\frac{T_{m,1}^{f} - T_{m,2}^{f}}{||r_{m,1} - r_{m,2}||} \quad F_m^{fs} = T_{m}^{f} - T_{m}^{s}
\]
The dual volumes at the boundary must be chosen according to the respective boundary condition as shown in Figures 12 and 13. With the use of the boundary co-occurrence matrices $\hat{d}_{i}^{3}$ and $d_{i}^{1b}$ and boundary values denoted by index $b$, the final PH system can be found:

$$\begin{bmatrix}
\dot{U}^s
\dot{U}^f
F^s
F^f
F^fs
\end{bmatrix}
=\begin{bmatrix}
0 & 0 & \hat{d}_i^{3} & 0 & I \\
0 & 0 & 0 & \hat{d}_i^{3} & -I \\
\hat{d}_{i}^{1} & 0 & 0 & 0 & 0 \\
0 & \hat{d}_{i}^{1} & 0 & 0 & 0 \\
-I & I & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
C^{-1} & 0 & 0 & 0 & 0 \\
0 & C^{-1} & 0 & 0 & 0 \\
0 & 0 & \Lambda^{s} & 0 & 0 \\
0 & 0 & 0 & \Lambda^{f} & 0 \\
0 & 0 & 0 & 0 & \alpha^{fs} \\
\end{bmatrix}
+\begin{bmatrix}
\dot{U}^s
\dot{U}^f
F^s
F^f
F^fs
\end{bmatrix}
=\begin{bmatrix}
0 & 0 & \hat{d}_i^{3} & 0 \\
0 & 0 & 0 & \hat{d}_i^{3} \\
\hat{d}_{i}^{1b} & 0 & 0 & 0 \\
0 & \hat{d}_{i}^{1b} & 0 & 0 \\
-I & I & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
T_{s}^b \\
T_{f}^b \\
T_{s}^{fs} \\
\end{bmatrix}
+\begin{bmatrix}
\dot{\Phi}_s^b \\
\dot{\Phi}_f^b \\
\end{bmatrix}
$$

5 Conclusion

In this paper we showed an approach to model heat transfer on open cell foams restricted to a cubic structure of the foam. We are currently working on the extension to an arbitrary structure, given by the tomography data.

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References

[1] V. Rosetti, Catalysts for H2 production, PhD Thesis, Università di Bologna, 2007.
[2] E. Brun and J. Vicente, imorph.
[3] J. P. Bonnet, F. Topin, and L. Tadrist, Transport in Porous Media 73(2), 233–254 (2007).
[4] J. M. Hugo, E. Brun, F. Topin, and J. Vicente, Defect and Diffusion Forum 297-301, 960–965 (2010).
[5] K. K. Bodla, J. Y. Murthy, and S. V. Garimella, Computational Materials Science 50(2), 622–632 (2010).
[6] V. Duindam, A. Macchelli, S. Stramigoli, and H. Bruyninckx, Modeling and Control of Complex Physical Systems (Springer, 2009).
[7] E. Tonti, Computer Modeling in Engineering and Sciences 2(2), 237–258 (2001).
[8] P. Alotto, F. Freschi, M. Repetto, and C. Rosso, The Cell Method for Electrical Engineering and Multiphysics Problems (Springer, 2013).
[9] M. Gerritsma, R. Hiemstra, J. Kreeft, A. Palha, P. Rebelo, and D. Toshniwal, The geometric basis of numerical methods, in: Lecture Notes in Computational Science and Engineering, (Springer, 2014), pp. 17–35.
[10] M. Pani and F. Taddei, Computer Modeling in Engineering and Sciences 94(4), 279–300 (2013).
[11] P. Kotyczka and B. Maschke, at-Automatisierungstechnik 65(5), 308–322 (2017).
[12] P. Kotyczka, Structured discretization of the heat equation: Numerical properties and preservation of flatness, in: 23rd International Symposium on Mathematical Theory of Networks and Systems, (Hong Kong, 2018), pp. 600–607.
[13] H. Flanders, Differential Forms with Applications to the Physical Sciences (Dover Publications Inc., 1989).
[14] A. N. Hirani, Discrete Exterior Calculus, PhD Thesis, California Institute of Technology, 2003.
[15] M. Seslija, J. M. A. Scherpen, and A. J. van der Schaft, Automatica 50(2), 369–377 (2014).