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RAREFIED GAS FLOWS THROUGH POROUS MEDIA DRIVEN BY PRESSURE AND TEMPERATURE GRADIENTS

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ABSTRACT

Pressure driven flows through porous materials [1] are encountered in many and diverse applications, including medical and biological flows [2], separation and filtration [3], catalytic convertors [4] and micro gas analyzers [5]. Furthermore, due to the increase of shale gas extraction, such flows are of interest to the petroleum industry [6]. In recent years, temperature driven flows through porous media have also gained considerable attention, due to the implementation of porous materials in the design of thermally driven Knudsen pumps [7-9].

Based on the local pore size the flow in porous media may be in a wide range of the Knudsen number and proper modeling is based on kinetic theory via the Boltzmann equation or a suitable kinetic model. It is evident that, due to the complex cross-section geometries of porous media, a solver able to handle geometries of arbitrary complexity is required. Most such rarefied gas dynamics solvers utilize typical numerical schemes, that require the solution of large systems of algebraic equations in each iteration [10-13]. An alternative, computationally more efficient approach, is the application of the so-called marching schemes [14].

Marching schemes do not require the solution of systems of linear equations. On the contrary the solution propagates in the direction of the molecular velocity, following a path such that when a computational node is considered all other nodes required for the solution propagation at this node have already been considered and their distribution function has been updated. Although computationally efficient, marching schemes have been limited to structured meshes, where obtaining this solution sequence is trivial based on the node indexing.

Here, an extension of marching schemes to unstructured meshes and its implementation in solving rarefied gas flows through porous media are presented. Two methodologies are developed for the calculation of the solution sequence, one based on purely geometrical arguments and another one based on a backtracking algorithm. The former is computationally efficient but can provide an erroneous path under certain conditions, while the latter is robust but computationally demanding.

In the geometrical method, consider a line normal to the molecular velocity vector sweeping through the flow domain. Since the distribution function propagates in the direction of the molecular velocity, when this line passes through a node, all other nodes required for the solution propagation have already been scanned by this line. The order according to which this line encounters the computational nodes is a valid solution sequence, when no obtuse elements exist.

In the backtracking algorithm, the solution sequence is incrementally built. It is initialized placing the boundary nodes with outgoing distributions in the first positions. Then the remaining nodes are considered

and when a node is found that has all nodes required for the solution propagation already placed in the solution sequence, it is appended to it, otherwise a different node is considered. This procedure is repeated until all the nodes of the computational mesh are placed in the solution sequence.

Based on the developed approach, the pressure and temperature driven flows through capillaries of fractal cross-sections are considered. Two fractal geometries are simulated: the Sierpinski carpet and the Apollonian gasket. The first four levels of the Sierpinski carpet and the first three levels of the Apollonian gasket along with indicative unstructured meshes are shown in Figures 1 and 2, respectively. The porosity (ratio of the void area over the total area) takes the values 1, 0.89, 0.79, and 0.7 for the level 0, 1, 2 and 3 Sierpinski carpets, respectively and 1, 0.7 and 0.65 for the level 0, 1 and 2 Apollonian gaskets, respectively. The numerical simulation is based on the infinite capillary approach using the Shakhov kinetic model equation [15]. Upon applying the normalization and projection procedures, the Shakhov model equation results in a system of two coupled integrodifferential equations for the two reduced distribution functions (φ_i and ψ_i), with the subscript $i = P,T$ denoting the pressure and temperature driven flows respectively. The system of equations used to model the rarefied gas flow through the capillaries of fractal cross-sections, is written in the following form

$$\zeta_x \frac{\partial \varphi_i}{\partial x} + \zeta_y \frac{\partial \varphi_i}{\partial y} = \delta \left[u_i + \frac{2}{15} q_i \left(\zeta_x^2 + \zeta_x^2 - 1 \right) - \varphi_i \right] + S_i^{\varphi}, \tag{1}$$

$$\zeta_x \frac{\partial \psi_i}{\partial x} + \zeta_y \frac{\partial \psi_i}{\partial y} = \delta \left[\frac{3}{4} u_i + \frac{1}{5} q_i \left(\zeta_x^2 + \zeta_x^2 \right) - \psi_i \right] + S_i^{\psi}, \tag{2}$$

where the macroscopic velocity $\left(u_i\right)$ and heat flux in the flow direction $\left(q_i\right)$ are given by

$$u_i = \frac{1}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \varphi_i e^{-\zeta_x^2 - \zeta_y^2} d\zeta_x d\zeta_y \quad \text{and} \quad q_i = \frac{1}{\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left[\varphi_i \left(\zeta_x^2 + \zeta_y^2 - 5/2 \right) + \psi_i \right] e^{-\zeta_x^2 - \zeta_y^2} d\zeta_x d\zeta_y, \tag{3}$$

while the source terms become

$$S_P^{\varphi} = -\frac{1}{2}, \; S_P^{\psi} = -\frac{3}{4}, \; S_T^{\varphi} = -\frac{1}{2}\left(\zeta_x^2 + \zeta_y^2 - 1 \right) \text{ and } S_T^{\psi} = -\frac{3}{4}\left(\zeta_x^2 + \zeta_y^2 \right). \tag{4}$$

The parameter characterizing the flow is the gas rarefaction parameter

$$\delta = \frac{PL}{\mu \upsilon_0}, \tag{5}$$

where P, L denote the reference pressure and length and μ, υ_0 the dynamic viscosity and most probable molecular speed at reference conditions. The kinetic equations (1) and (2) are discretized using the Discrete Velocity Method (DVM) [14-16] for the molecular velocity space discretization, while the physical space is discretized using an unstructured triangular mesh. Upon solving the kinetic equations, the velocity profile is obtained and the reduced flow rate is calculated as

$$M_i = 2 \int_A u_i dA. \tag{6}$$

The ability of the developed methodology to accurately simulate rarefied gas flows in arbitrary geometries using unstructured meshes is demonstrated comparing the obtained reduced flow rate for the pressure driven flow with the results of [17] for the Sierpinski carpet and of [11] for the Apollonian gasket. The comparison is presented in Figure 3 for the Sierpinski carpet (left) and for the Apollonian gasket (right). In both cases, the present results are in excellent agreement with the results existing in the literature. Moreover, quantities of practical interest can be readily extracted, such as the apparent permeability $\left(k\right)$. The apparent permeability, calculated at $\delta = 10$, takes the values 3.2×10^{-2}, 1.4×10^{-2}, 6×10^{-3} and 2.2×10^{-3} for the level 0, 1, 2 and 3 Sierpinski carpets, respectively and 2.8×10^{-2}, 4.3×10^{-3} and 2.7×10^{-3} for the level 0, 1 and 2 Apollonian gaskets, respectively. Using the present methodology, more complicated flow configurations, including actual porous media geometries can be studied accurately and in a computationally efficient manner.

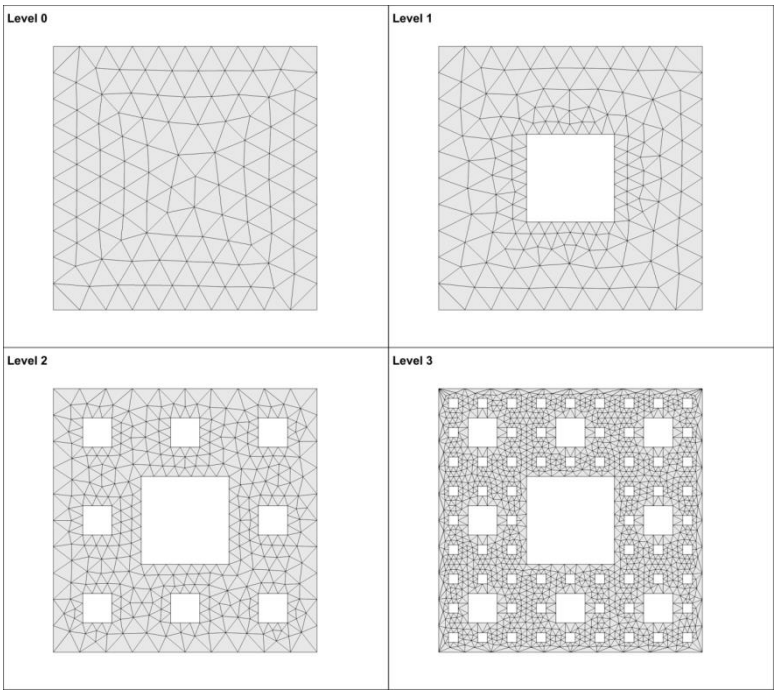

Figure 1: First four levels of the Sierpinski carpet fractal along with indicative meshes.

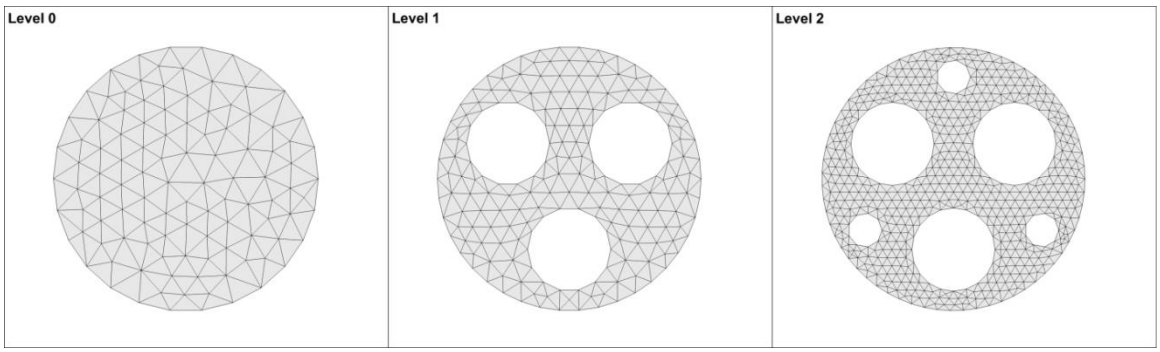

Figure 2: First three levels of the Apollonian gasket fractal along with indicative meshes.

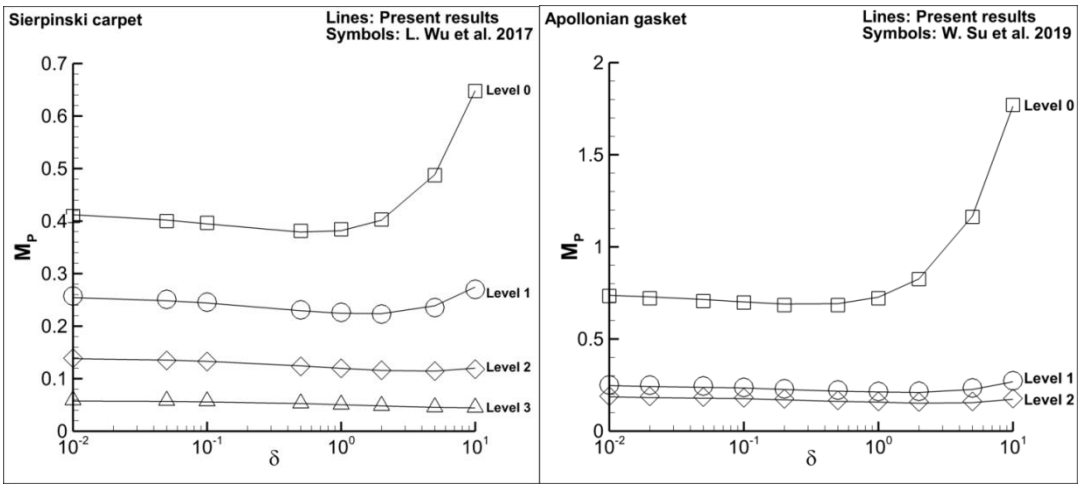

Figure 3: Reduced flow rate in terms of δ for the Sierpinski carpet (left) and Apollonian gasket (right).

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