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DIRECTED HIERARCHICAL SELF ASSEMBLY – ACTIVE FLUID MECHANICS AT THE MICRO AND NANOSCALES

Mekala Krishnan
Sibley School of Mechanical and Aerospace Engineering,
Cornell University, Ithaca, New York, 14853

Michael T. Tolley
Sibley School of Mechanical and Aerospace Engineering,
Cornell University, Ithaca, New York, 14853

Hod Lipson
Sibley School of Mechanical and Aerospace Engineering, Computing and Information Science,
Cornell University, Ithaca, New York, 14853

David Erickson
Sibley School of Mechanical and Aerospace Engineering,
Cornell University, Ithaca, New York, 14853
de54@cornell.edu

ABSTRACT

Directed hierarchical self assembly (DHSA) involves the purposeful assembly of a series of different subunits over multiple length scales to create arbitrarily shaped, large structures. We are developing a two stage DHSA procedure comprising of a coarse "far field" fluidic process which brings the sub-elements into the general vicinity of the assembly point and a fine "near field" process which completes the process. In the experiments presented here our sub-elements comprise of lithographically patterned silicon "microtiles" which are 500µm in size and contain a series of functional elements. The far-field assembly of these tiles is controlled fluid dynamically by modulating the translational and rotational shear forces applied to the tiles with a microfluidic structure. The near-field assembly is controlled through on board (*i.e.* on tile) microchannel jets/sinks, the strengths of which are modulated through the assembly or disassembly of thermally actuated gel based microvalves. This provides two fundamental levels of system control, namely control of the magnitude and direction of fluid flow, as well as addressability and control of each assembled component through on tile valves. In this paper we present our preliminary work on the fundamental fluid mechanics of this assembly at these two stages. In the first section we look at fluid motion and forces using CFD based numerical simulations. In the second we study a valving system based on an aqueous solution of a triblock copolymers that form a gel at temperatures near room temperature.

INTRODUCTION

Figure 1 is a schematic showing our approach to directed fluidic self assembly. The chamber (a modified version of which will be described in greater detail later) contains a series of microchannel inlets and outlets arranged along an assembly substrate. As mentioned in the abstract, in our envisioned system each tile will also have on board microvalves which allow us to control the near field assembly process. Previously we have demonstrated the manipulation and far-field assembly of 500µm silicon microtiles [1]. As an example of this, Figure 2 illustrates the assembly of two tiles by selectively opening and closing of valves along the assembly substrate.

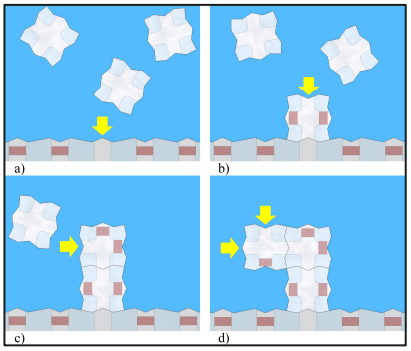


Figure 1: Assembly of tiles using fluidic forces
Tiles are manipulated by fluidic forces, and are controlled and addressed by an on-board valving system.

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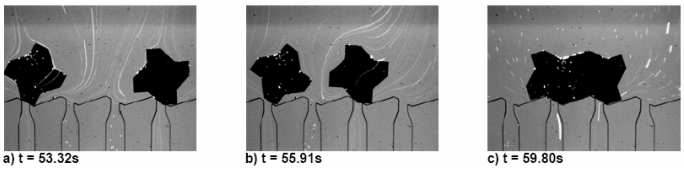


Figure 2: Multi-tile assembly on a substrate [1]

In this paper we will provide an overview of our recent progress towards developing an integrated far-field, near-field assembly process. In the first half we summarize of efforts on modeling the far-field process using CFD. The second section covers our efforts to build an on-tile valving structure and use it to control the near field assembly process.

FAR FIELD ASSEMBLY - FLUIDIC CONTROL

Microfluidically driven assembly of the tiles tiles requires an understanding of the forces and torques that moving fluid can exert on a floating body. Here, we carry out a numerical analysis of our tile system and demonstrate controlled motion of tiles by fluidic actuation. Broadly speaking moving fluid exerts both a force and a torque on a solid body in the fluid, resulting in displacement of the body. This in turn affects the flow field around the body. Hence, a coupling exists between the flow field and the motion of the body. We describe the motion of the fluid using the 2 dimensional, incompressible Navier Stokes equations for a Newtonian fluid,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u} \quad (1)$$

$$\nabla\cdot\mathbf{u} = 0 \quad (2)$$

where $\mathbf{u}$ is the velocity of the fluid, p is the pressure, and ρ and ν are the density and viscosity of the fluid respectively.

The force, $\mathbf{F}$ and torque, $\mathbf{T_B}$ on the body are computed using the stress tensor, $\boldsymbol{\tau}$, such that

$$\mathbf{F} = \int_A (\boldsymbol{\tau}\cdot\mathbf{n})dA \quad (3)$$

$$\mathbf{T_B} = \int_A (\mathbf{r}\times(\boldsymbol{\tau}\cdot\mathbf{n}))dA \quad (4)$$

where A is the surface of the body, and $\mathbf{n}$ is the surface normal. $\mathbf{T_B}$ refers to the torque with respect to the body co-ordinates.

The force and torque on the body can be used to obtain the linear and angular acceleration of the tile. The new position of the tile can be found from this acceleration using a first order Eulerian discretization scheme. Once the updated position of the tile is obtained, the new flow field is calculated and the above process repeated. We have used the commercial software FLUENT to carry out these simulations. Our simulations have demonstrated the assembly of programmable structures using fluidic forces to manipulate and position tiles. Figure 3 shows the results of fluidic simulations assembling a 'C' structure.

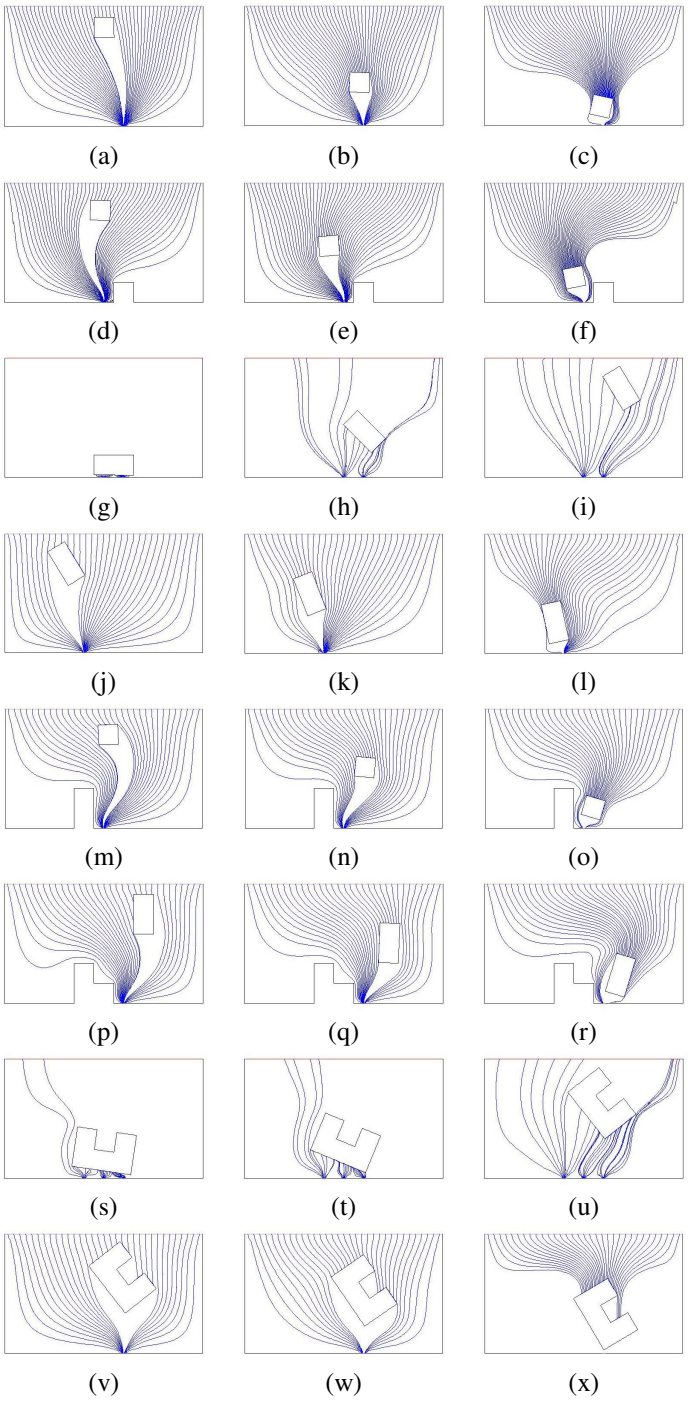


Figure 3: Demonstration of multi-tile assembly using fluidic forces (a-c) show a fluidic simulation of a single tile being pushed down in the chamber by fluid moving towards an open outlet, while (d–f) show the assembly of a two tile system. Panels (g-i) show the straightening and release of a latched two tile system from the substrate. (j–x) show the remaining assembly steps towards the formation of a 'C'.

Deterministic and in particular low error assembly of microtiles onto a substrate requires that tile orientation at the

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time of assembly be predictable and controllable. In order to study this, we have carried out a series of numerical experiments looking at the "docking" behavior of different tile shapes on a substrate with different outlet configurations. The different tile shapes studied were a) Square tiles (both with and without valves) b) Hexagonal tiles c) Octagonal tiles. Table 1 gives the details of the different shapes used and their dimensions. Additionally, we looked at the effect of number of outlets on tile orientation. Similar work on the orientation of differently shaped assembling units has been carried out [3] for fluidic self assembly based on capillary action.

Table 1: Different tile shapes studied

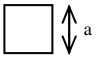
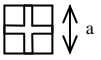
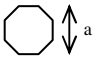
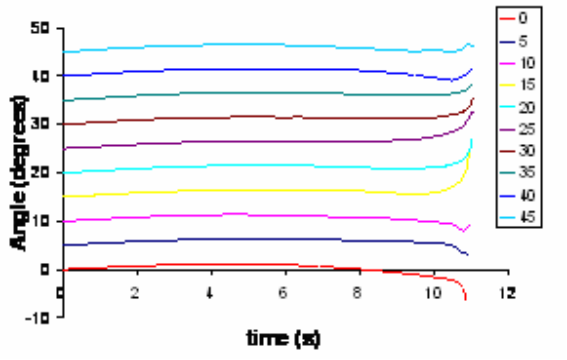
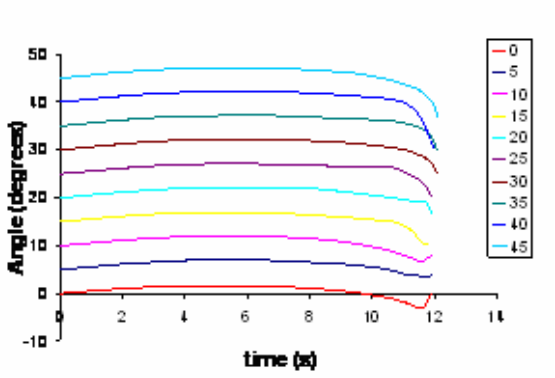
Name	Shape	Dimension (μm)
Square (without valve)		a = 500 μm
Square (with valve)		a = 500 μm (slot size = 50 μm)
Regular Hexagon		a = 500 μm
Regular Octagon		a = 500 μm

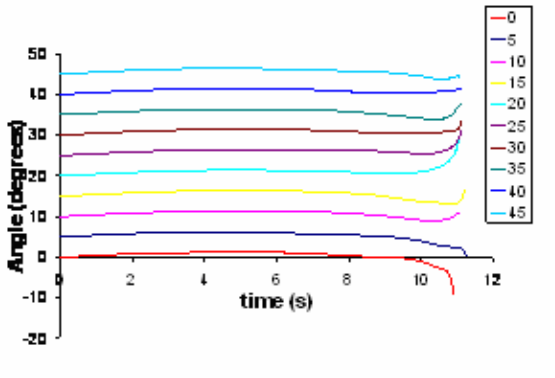
Figure 4 shows the variation in tile orientation with time as the tile moves across the chamber for different tile shapes and outlet configurations. The legends in the figures refer to initial tile angles with respect to the substrate of the chamber. It was found that a dual outlet set up worked well on the square tiles, both with and without valves, and caused the rotation of the tile to correct such that the final angle tended towards zero, regardless of the initial orientation (see figures 4b, d). This effect was less evident in the hexagonal and octagonal tiles, possibly because of the increased number of sides in these shapes as compared to squares.



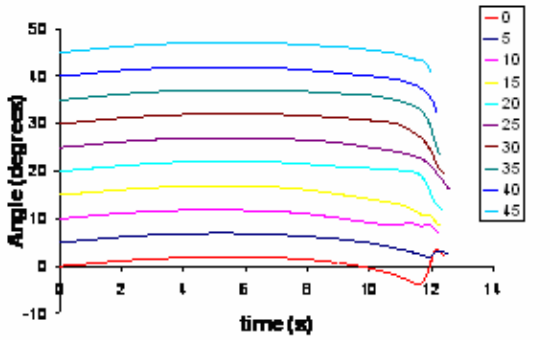
(a)



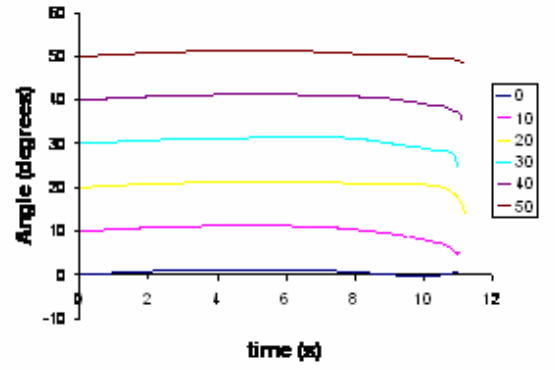
(b)



(c)

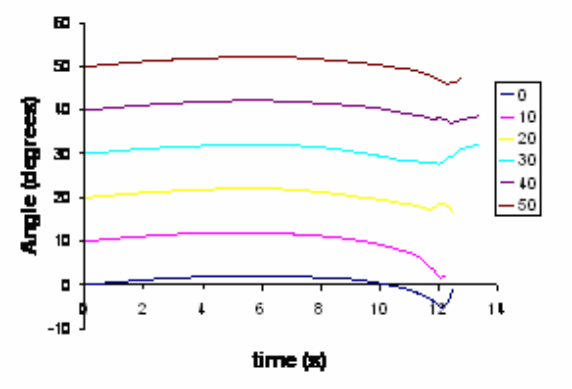


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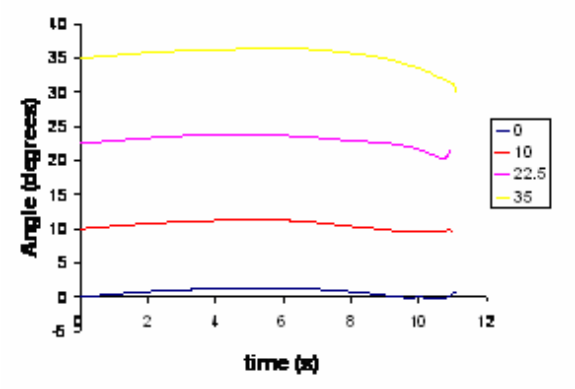


(e)

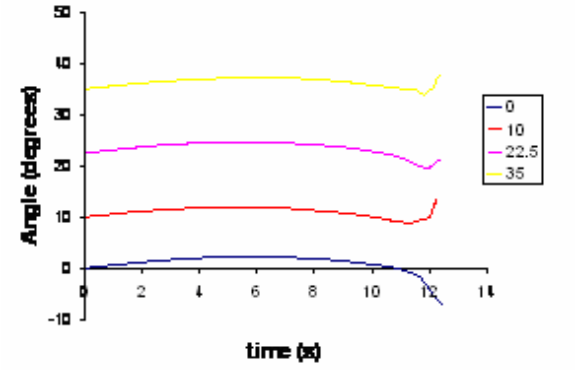
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(f)



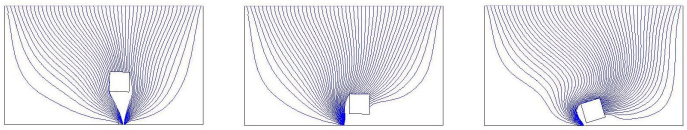
(g)



(h)

Figure 4: Tile orientation for different tile shapes and initial angles (a) Square tile without valves with single open outlet (b) Square tile without valves with two adjacent open outlets (c) Square tile with valves with single open outlet (d) Square tile with valves with two adjacent open outlets (e) Hexagonal tile without valves with single open outlet (f) Hexagonal tile with two adjacent open outlets (g) Octagonal tile with single open outlet (h) Octagonal tile with two adjacent open outlets

Another assembly scheme we looked at consisted of tile assembly by sequential opening and closing of outlets. Figure 5 demonstrates the assembly of a square tile on a substrate by first opening one outlet, and subsequently closing it while opening the outlet adjacent to it. This allows for good control over tile positioning, as can be seen in the figure.



(a) (b) (c)

Figure 5: Tile manipulation by sequential opening and closing of outlets (a-c) A tile is manoeuvred between two outlets by first opening one outlet and then the outlet adjacent to it

NEAR FIELD ASSEMBLY – THERMALLY ACTUATED GEL VALVES

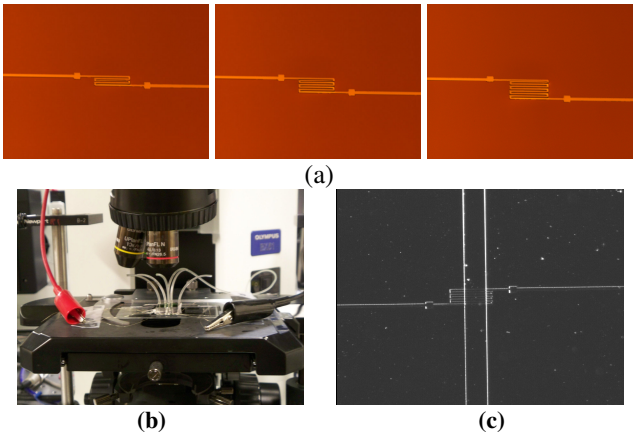
As mentioned above, the "near field" assembly of the tiles in the microfluidic chamber is controlled through on board (i.e. on tile) microchannel jets/sinks, the strengths of which are modulated through the assembly or disassembly of thermally actuated gel based microvalves. The on board integration of these valves on the tiles will provide us with the ability to control the near field assembly of the tiles, as well as assemble subsequent layers of tiles above those assembled on the chamber substrate.

The valving system we are working on is based on previous work on copolymer based microvalves [2]. The copolymer used here is a water soluble, symmetric triblock copolymer consisting of poly(ethylene oxide)$_x$ – poly(propylene oxide)$_y$ – poly (ethylene oxide)$_x$ or PEO$_x$ – PPO$_y$ - PEO$_x$. An aqueous solution of this copolymer exhibits reversible sol-gel transition on heating. The temperature at which the transition occurs varies depending on the concentration of the solution [4]. When an aqueous solution of the copolymer is heated to its transition temperature, it becomes an elastic gel with a yield stress. This phenomenon can be used to design valves in which flow through a channel is shut off due to heating and subsequent gelation of the solution in that channel. Flow through the channel resumes once the gel cools below the transition temperature and becomes an aqueous solution again. The copolymer used in our experiments is PEO$_{106}$ – PPO$_{70}$ – PEO$_{106}$ which has the trade name Pluronic® F127. This is a commercially available material that was obtained from BASF. The advantage of using this material is that its gel transition temperature lies close to room temperature for solution concentrations in the range of 15-20 % by weight [4]. As a result, the amount of heat needed for gelation is not very high, and can be provided by lithographically patterned platinum heaters. We tested solutions ranging from 5-20 % for our experiments and found that the 15 % solution worked best, as it was relatively easy to pump through the channel, as well as heat to its gel transition state.

Our experimental set up to test the working of these valves consists of microchannels with platinum heaters. A silicon wafer

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was initially coated with 1 μm of silicon dioxide using plasma enhanced chemical vapour deposition (PECVD) to insulate the heaters from the wafer. Platinum heaters and electrodes (150 nm) were then patterned on the wafer by lift off processing using a titanium adhesion layer (30 nm). An insulating layer of 500 nm thick silicon nitride was deposited on the wafer by a PECVD process, followed by a selective RIE etch of the nitride to expose the bonding pads on the electrodes and allow interfacing of the external electronics. Finally, a 10 micron thick PDMS mold of the fluidic channels was made using an SU-8 master. The silicon wafer and the PDMS channels were both plasma cleaned and bonded together. The final chip was left overnight in a convection oven at 80°C to ensure complete bonding. The experimental set up consists of different heater coil dimensions and channel widths ranging from 5 μm to 100 μm. The heater coils were 5 μm wide and ranged from 5 to 9 strips that ran across the channels. Figure 6 shows optical images of the different heaters used, the apparatus used for these experiments and an optical image of the heater coils beneath a microchannel.



(a)

(b) (c)

Figure 6: Experimental set up (a) Different heater coils used in the experiments (b) Apparatus used to carry out experiments of gelation in a microchannel (c) Optical image of platinum heater coils beneath a PDMS based microchannel

Fluid pressures ranging from 1 to 10 psi were used to pump the Pluronic solution through the microchannels. Flow through the channel was visualized using fluorescent particles of 1.9 μm diameter. As expected, fluid flow was faster in the wider channels as compared to the narrow ones at the same pressure due to their lower hydraulic resistance. In general, it was found that the longest heater coil worked best. Gelation was found to occur instantaneously for inlet pressures in the range of 1-2 psi for applied voltages of 25-30V. On applying this voltage, flow through the channel was found to come to a complete stop. Flow resumed on turning the power supply to the heaters off, though it took some time (5-10s) for the flow to return to its original speed. Application of lower voltages (~ 15-20V) was found to slow the flow rate in the channel, but did not cause the flow to stop, even after 20-30s of heating.

The next step towards the on chip integration of these valves is to test them in a fluidic chamber similar to the one used in [1]. In order to do this, we are modifying the chamber used there to include PDMS 'tiles' on the substrate of the chamber with channels through them. Figure 7 is a CAD rendering of this, showing the fluidic chamber with PDMS tiles.

The PDMS will be bonded on to a pyrex wafer, with patterned platinum heaters on the wafer similar to the ones used in the previous experiments (Corning 7740). The fluid flowing through the chamber will be a 15 % pluronic solution, and the heaters on the pyrex base of the chip will serve to selectively valve the channels on the PDMS tiles.

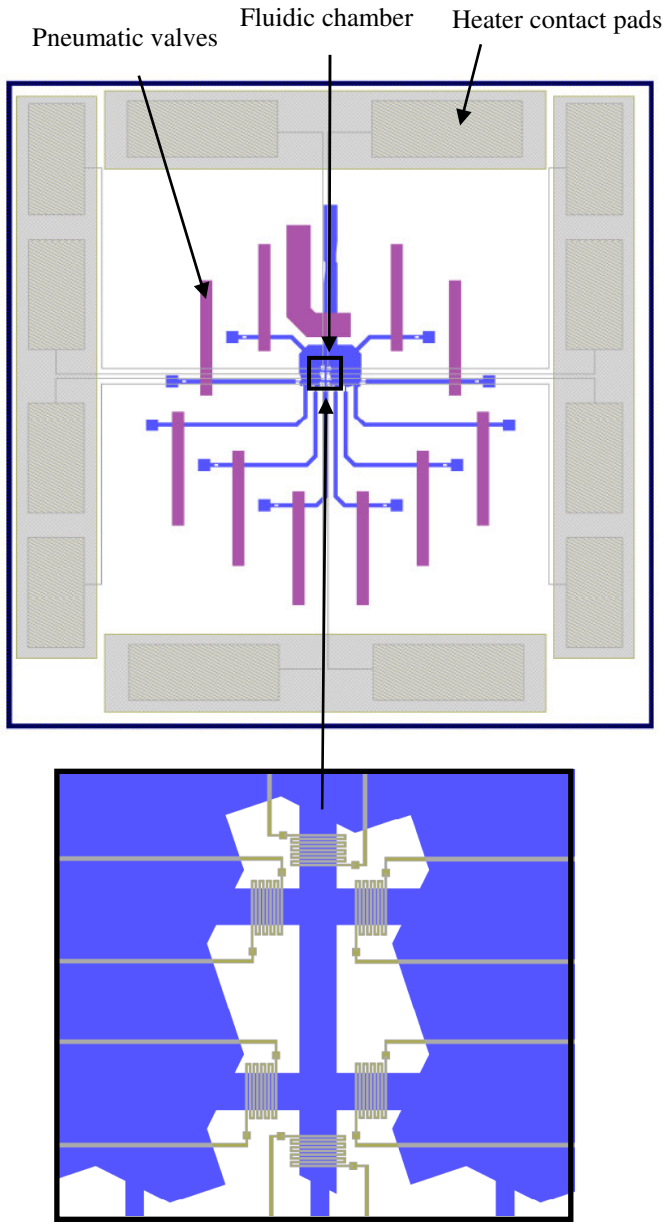


Figure 7: CAD image showing PDMS chamber with heaters and contact pads

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ACKNOWLEDGMENTS

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