A Computational Framework For Modeling One-Dimensional, Sub-Grid Components And Phenomena In Multi-Dimensional Microsystems

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ABSTRACT

This paper presents a framework for modeling essentially one-dimensional devices and components embedded in multi-dimensional spaces. The main characteristic and main advantage of the new methodology is that the one-dimensional and multi-dimensional objects or domains are meshed completely independently of each other, without regard to their relative alignment or location, and subsequently combined into a single, unified composite mesh. The coupling of the solution between the different domains is handled fully-automatically in the solver, entirely through exchange of source terms between these domains of differing dimensionality. The source terms are evaluated locally on a cell-by-cell basis, depending on the solution values in these domains and the manner in which the one-dimensional grids intersect the multi-dimensional grids. The capabilities and usefulness of the method are demonstrated with several examples.

Keywords: filament, fiber, computational models, sub-grid models, reduced models.

1 INTRODUCTION AND BACKGROUND

Microsystems frequently contain embedded objects or components that are pre-dominantly one-dimensional, i.e., long and slender and with transverse length scales that are much smaller than the isotropic length scales of the multi-dimensional space in which the objects are embedded. Examples include microchannels in fluidic devices, optical or electrical leads or other conducting paths in micro-chips, and waveguides and antennas in open spaces. Such one-dimensional objects are here called filaments. The main practical challenge in computational modeling of such systems is in overcoming the mesh generation difficulties caused by the large differences in length scale. Another major undesirable effect of traditional approaches to meshing problems with widely disparate length-scales arises from the need to maintain grid matching across the different domains, forcing the length-scales of cells in the multi-dimensional domain surrounding the filaments to be comparable with the length-scales of cells in the filament domain. This can unnecessarily increase the total number of cells in the multi-domain problem by several orders of magnitude.

This paper presents a generic, efficient, automated computational framework, called the "filament" model, recently developed in the multi-physics computational simulation tool, CFD-ACE+, for accurately and comprehensively modeling such multi-domain, multi-scale problems.

2 MODELING APPROACH AND IMPLEMENTATION

The modeling approach adopted in this work relies on meshing the filaments and the embedding regions completely independently, using whatever is the most efficient mesh generation technique for each. Typically, the multi-dimensional domains are meshed using either structured, unstructured, or hybrid grids. Unstructured grids may be of the tetrahedral, prismatic, Cartesian, or arbitrary polyhedral type. The filament structures are meshed in a fully-automated manner as a string of single-celled elements, as shown in Figure 1 below.

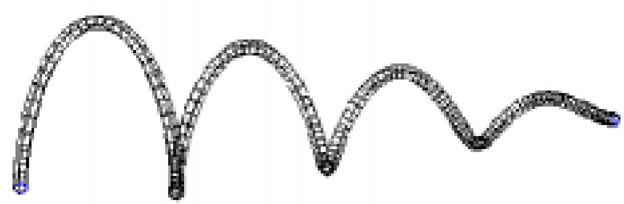

Figure 1: Example of an individual filament structure and its grid.

The filament grids are then embedded into the multi-dimensional grid without any regard to alignments or mismatches between the filament and multi-dimensional grids. The intersection pattern between the one-dimensional filament meshes and the multi-dimensional meshes is then determined. This is done by computing the intersections of the filament center-lines (which are allowed to trace arbitrary paths in the domain) with the multi-dimensional mesh, using an efficient ray-tracing algorithm. The full geometric description of the individual filament segments that lie inside each intersected cell of the multi-dimensional domain, including the surface areas and volumes of the segments are also computed. Figure 2 below shows an example of filament embedding in a multi-dimensional domain.

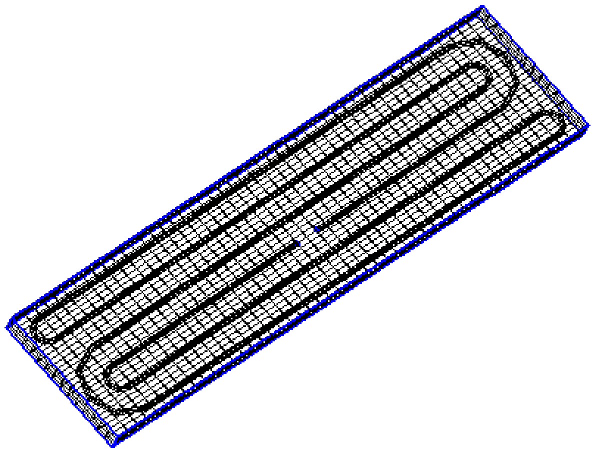

Figure 2: Example of a filament structure representing a heating coil, embedded in a three-dimensional region representing the heated space in an oven.

The filament approach requires the transverse dimensions of filaments to be much smaller than the dimensions of the cells of the multi-dimensional grid through which these filaments pass. The blockage effect of filament segments on flow or other transport phenomena is also accounted for by modifying the volumes and face areas of the intersected cells of the multi-dimensional grid. The slenderness assumption greatly simplifies the geometry calculations, including the determination of intersections and the calculation of blockage effects. The complete description of the geometries of the filament segments and the cells with which they are associated are stored in appropriate data-structures.

The governing equations in all the one-dimensional and multi-dimensional domains are solved simultaneously, using an implicit, iterative, segregated solution methodology [1]. The same solvers and boundary procedures are used for all the domains (i.e., for the computational cells in the filaments and the computational cells in the multi-dimensional embedding spaces). The coupling between the solutions in the independently-meshed domains of differing dimensionality is imposed on the overall solution entirely through the two-way exchange of mass, momentum, energy, or other source and sink terms. The source and sink terms are typically evaluated using standard transfer correlations that are computed locally for each cell through which a filament passes. The typical form of the transfer equation is given by:

$$\dot{q} = hA_f \Delta\phi \qquad (1)$$

where $\dot{q}$ is the exchange rate of the quantity ϕ between cell c of the multi-dimensional grid and the filament segment passing through that cell, h is an empirical or theoretical coefficient for the exchange rate, A_f is the surface area of the filament segment passing through cell c, and $\Delta\phi$ is the difference between the values of ϕ in the filament segment and the cell c, $\Delta\phi = \phi_c - \phi_f$, where ϕ_c and ϕ_f are respectively the values of property ϕ in cell c and the filament segment passing through that cell. Other transfer models may also easily be used instead, and the forms of the transfer equations for mass, momentum, and energy, or any other variable, can be independently programmed or selected by the user.

3 USER INTERFACE AND MODEL PREPARATION

The background grid is created using CFD-GEOM, the Geometric Modeling and Grid Generation package used with CFD-ACE+, as described in [2]. Filament grids are created using a separate GUI-driven preprocessor, consisting of a simple window, and using intuitive, simple commands. The window and the filament construction procedure are shown in Figure 3 below.

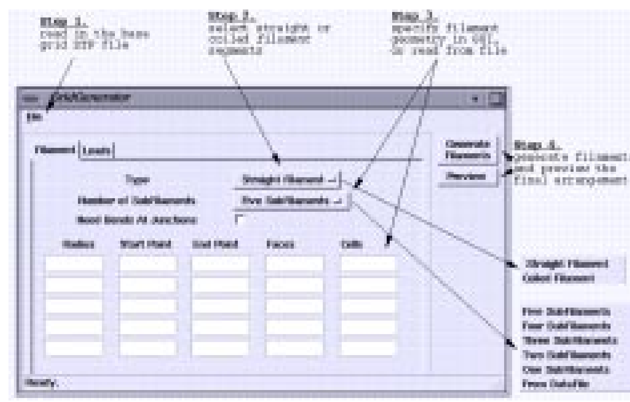

Figure 3: The GUI window for specification and meshing of filaments.

4 VALIDATION AND DEMONSTRATION

This section presents the results of three simulations which illustrate the utility of the filament approach to problems having the following features: large disparity in geometrical scales, multi-disciplinary phenomena, and domain-domain interactions.

4.1 Case 1. Disparity of Geometrical Scales

Figure 4 shows the temperature distribution for filament heating in a microfluidic reactor to promote reaction kinetics. The filaments model five heating elements embedded in, and heating the wall of the main reactor channel as shown. The thermal energy is then passed to the fluid, activating the reaction. Typical length scales associated with the simulation are 500μm for the channel and 0.1μm for the filament. Because of the disparity in the length scales, conventional meshing techniques would produce prohibitively large meshes.

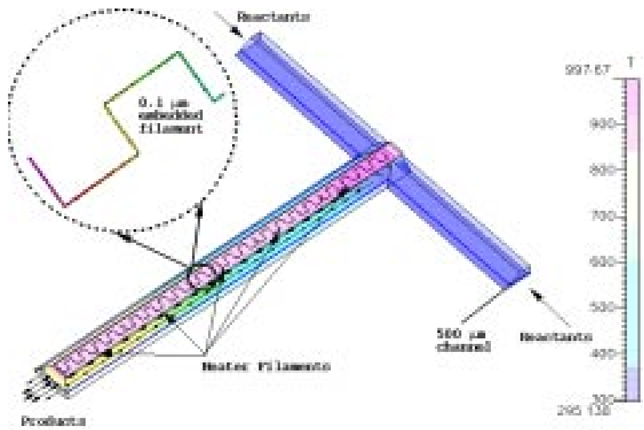

Figure 4: Filament heating in micro-fluidic reactor.

4.2 Case 2. Multi-Disciplinary Phenomena

Figure 5 shows the temperature distribution for filament heating of swirling flow in a cylinder. The filament models a resistance coil energized through Ohmic heating. The filament embedding process effectively creates a single unstructured virtual domain composed of the multi-dimensional as well as the filament grids. Since the filaments now form an integral part of the computational domain, any physical model available within CFD-ACE+ can be used in any part of the domain for simulation of multi-disciplinary phenomena. In this particular case, the Navier-Stokes equations were solved to calculate the flow heating on the multi-dimensional (cylinder) grid, and electrostatic field equations were solved to calculate the Ohmic heating in the filament coil.

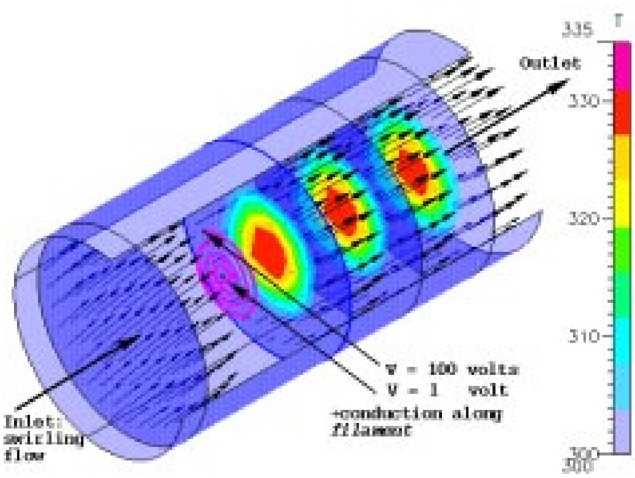

Figure 5: Filament-based Ohmic heating of swirling flow.

4.3 Case 3. Domain-Domain Interaction

Figure 6 shows the use of filaments in a cooling simulation of a heated microchip mounted on a pedestal heat sink. The chip and pedestal are modeled as two separate computational domains. Figure 6a shows the initial system geometry as well as the temperature distribution. Since the two domains are physically separated by a thin air gap, and since radiation effects are ignored, only convective heat transfer occurs between the chip and the pedestal. Figure 6b shows the effect on the temperature distribution of introducing forty-eight filaments to join the two domains.

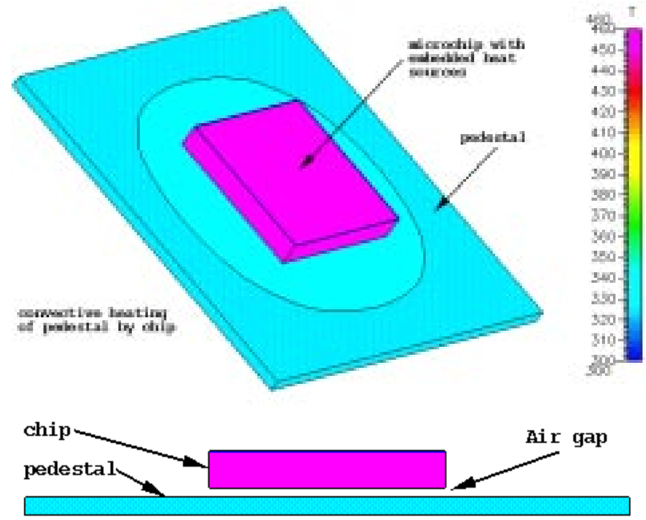

Figure 6a: System geometry and convective heat exchange between the separated chip and pedestal domains.

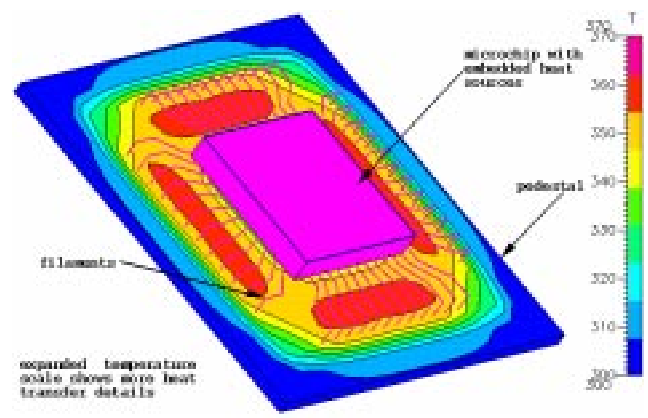

Figure 6b: Conduction heat exchange between the filament-joined domains.

The simulation clearly illustrates that the heat flow between the two domains is dominated by the conduction along the filaments. Note the change in temperature scales between Figures 6a and 6b. "Filament embedding" boundary conditions were used, requiring the filament tip temperatures to be same as those in the domains to which they are attached. Again, for illustrative purposes, constriction thermal resistance effects were ignored. It can be seen that the meshing of this problem using conventional techniques would lead to a large increase in the total number of computational cells.

5 SUMMARY AND CONCLUSIONS

A framework for modeling essentially one-dimensional phenomena embedded in multi-dimensional spaces has been implemented as a separate module in the multi-physics simulator, CFD-ACE+. The main characteristic and main advantage of the new methodology is that the one-dimensional and multi-dimensional objects or spaces are meshed completely independently without any regard to mis-matches in alignment or location of the filaments in the multi-dimensional grid, and the coupling between the different domains is handled fully-automatically in the solver. The main restriction for accurate use of the filament module is that the filaments must be slender compared to the cells in which they are embedded. The feasibility and utility of the computational technique have been demonstrated, and its savings in turn-around time for both the meshing and analysis tasks have been indicated.

6 REFERENCES

[1] CFD Research Corporation, CFD-ACE(U): Version 6.0, February 2000.

[2] CFD Research Corporation, CFD-GEOM: Version 6.0, February 2000.