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Heat Transfer LES Simulations in Application to Wire-Wrapped Fuel Pins

Yulia Peet [1 2 *] and Paul Fischer [1 †]

[1] *Mathematics and Computer Science Division, Argonne National Laboratory*

[2] *Department of Engineering Sciences and Applied Mathematics, Northwestern University*

We present a novel development of a domain decomposition method for the Navier-Stokes equations in a spectral element formulation which enables to investigate turbulent flows in complex geometries. The current paper applies domain decomposition method to simulate turbulent heat transfer in a wire-wrapped fuel pin assembly. The method is first validated on a benchmark problem of a turbulent swept flow over a single wire in a channel. Potential application of the method to simulation of a realistic wire-wrapped assemblies is the discussed.

I. Introduction

Wire-wrapped fuel pin assemblies represent a coolant system for next generation advanced burner fast reactors. The liquid coolant flow passes through subassemblies of hexagonally arrayed fuel pins. Fuel pins are supported by a wire wrap spacer which wounds helically along the pin axes. In addition to providing a structural support, wire wrap also serves to promote a turbulent mixing of the coolant flow in order to increase the heat transfer coefficient and enhance cooling of the fuel pin walls.

Analysis of the flow and heat transfer properties in the described configuration presents significant challenges, due to both geometrical complexity and high Reynolds number of the coolant flow ($Re_h \sim 40000 - 65000$ based on hydraulic diameter of the subchannels). Geometrical complexity manifested by the presence of multiple contact points and lines due to the wire wrap makes it practically impossible to create body-fitted structured hexagonal mesh of the exact geometry required by the computational solver. Thus, previous computational investigations of wire-wrapped fuel pins performed at Argonne National Laboratory[1–3] used approximated rather than exact geometry of a subassembly, where the singularity line representing a line of contact between the wire and the pin was artificially smoothed out in order to enable mesh generation. Unfortunately, this singularity line is the most critical place in terms of cooling considerations, since a hot spot can be generated there due to stagnation flow conditions.

Special computational methodology was developed in order to facilitate mesh generation procedure and allow for the exact geometrical representation of the given problem. This methodology, consisting of assembling overlapping grids and performing unsteady interface conditions exchange was implemented in a stable and accurate manner in a spectral element solver NEK5000. With this methodology, an accurate meshing of the wire-wrapped fuel pin with two overlapping subdomains becomes possible, so that the computations of heat transfer in a wire-wrap configuration can be performed. After brief description of essential features of NEK5000 in Section II, computational methodology of the domain decomposition procedure is presented in Section III, the validation of the procedure on a benchmark problem of a turbulent swept flow over a single wire in a channel is described in Section IV, and potential application of the method to simulation of wire-wrapped fuel pin assemblies is discussed in Section V.

*E-mail: peet@mcs.anl.gov

†E-mail: fischer@mcs.anl.gov

II. Numerical Method

Spectral element code NEK5000[4] is used for performing Large Eddy Simulations (LES) of a heat transfer in a wire-wrapped fuel pin. Spectral element method (SEM) is a high-order weighted residual technique that combines the geometric flexibility of finite elements with the rapid convergence and tensor-product efficiencies of global spectral methods. Time discretization uses explicit backward-differentiation for convective terms, and implicit Crank-Nicolson scheme for viscous terms. Spatial filter removing energy from the highest modes developed in Ref. 5 serves as a hyperviscosity SGS model for the LES. Incompressible Navier-Stokes equations together with the transport equation for the temperature are solved in a fluid domain, and a time-dependent heat transfer equation is solved in a solid domain in a current conjugate heat transfer simulation. Current algorithm was optimized to achieve perfect scalability in parallel implementation up to 131,072 processors[1] and was successfully applied to perform Large Eddy Simulation of turbulent diffusion in 217-pin wire-wrapped sodium fast reactor fuel assemblies featuring about 3 million elements and about 1 billion of total grid points on 32,768 quad-core compute nodes on IBM Blue Gene/P at the Argonne Leadership Computing Facility.[3]

III. Domain Decomposition

In order to resolve the flow and heat transfer in the vicinity of the intersection between the wire and the fuel pin in a fuel pin assembly (see Figs. 8, 9), a new capability had to be implemented in the numerical solver: a capability of having several overlapping domains with their own geometrical topology coupled into a single simulation through the real-time exchange of interface values. This domain decomposition capability greatly enhances the ability of the solver to handle complex geometries and simplifies the mesh generation process. In addition, it gives the flexibility of local clustering of grid points in the places with sharp gradients of the flow variables without sacrificing the global structure of the mesh.

In a spectral element formulation, the computational domain Ω is subdivided into nonoverlapping subdomains, or elements, $\Omega = \cup_{k=1}^{K} \Omega_k$. Each Ω_k is the image of the reference subdomain under a mapping $\boldsymbol{x}^k(\boldsymbol{r}) \in \Omega_k \rightarrow \boldsymbol{r} \in \hat{\Omega}$, with a well-defined inverse $\boldsymbol{r}^k(\boldsymbol{x}) \in \hat{\Omega} \rightarrow \boldsymbol{x} \in \Omega_k$, where the reference subdomain $\hat{\Omega} = [-1, +1]^d$. Scalar functions within each element Ω_k are represented in terms of tensorproduct polynomials on a reference subdomain $\hat{\Omega}$, which, for example, in two dimensions looks like

$$f(\boldsymbol{x})|_{\Omega_k} = \sum_{i=0}^{N} \sum_{j=0}^{N} f_{ij}^k \, h_i(r_1) \, h_j(r_2), \;\; r_1, r_2 \in [-1, +1]^2, \tag{1}$$

where $h_i(r)$ is the Lagrange polynomial of degree N satisfying $h_i(\xi_j) = \delta_{ij}$, δ_{ij} is the Kronecker delta function, and $\xi_j \in [-1, +1]$, $j = 1, \ldots, N$ are the Gauss-Lobbato Legendre (GL) quadrature points.

When several overlapping domains are considered, if the domain Ω^i intersects the domain Ω^j, the boundary of the domain Ω^i which is within Ω^j, Γ^{ij}, needs to receive the values from the domain Ω^j to set as boundary conditions at this boundary, and the boundary of the domain Ω^j which is within Ω^i, Γ^{ji}, needs to receive the values from Ω^i. For the case of two domains, it is schematically illustrated in Fig. (1). Therefore, the main task is to find the values of each function $f(\boldsymbol{x})$ in the domain Ω^j at the points $\boldsymbol{\xi}^i \in \Gamma^{ij}$ (and in the domain Ω^i at the points $\boldsymbol{\xi}^j \in \Gamma^{ji}$), which are the GL points of the domain Ω^i (Ω^j) lying on the interface boundary Γ^{ij} (Γ^{ji}), at each computational (and each sub-iteration) time step.

In the spectral element formulation, once the element Ω_k^j of the domain Ω^j containing the boundary point $\boldsymbol{\xi}^i \in \Gamma^{ij}$ is identified, and the local coordinates $(r_1(\boldsymbol{\xi}^i), r_2(\boldsymbol{\xi}^i)) \in [-1, +1]^2$ are found, the **exact** value of the spectral approximation function $f(\boldsymbol{x})$ given by Eq. (1) will be obtained at the point of interest $\boldsymbol{\xi}^i \in \Gamma^{ij}$. It means that interpolation errors are absent in the spectral element formulation, unlike in finite difference methods, where they can be the large source of errors. The task of locating the element Ω_k^j containing the point $\boldsymbol{\xi}^i \in \Gamma^{ij}$ is performed by testing the relative location of the point with respect to the bounding box associated with each element. Once the element containing the point is located, the problem of finding the corresponding local coordinates $(r_1(\boldsymbol{\xi}^i), r_2(\boldsymbol{\xi}^i)) \in [-1, +1]^2$ is cast into an optimization problem which minimizes the value of $|\boldsymbol{\xi}^i - \boldsymbol{x}(\boldsymbol{r})|^2$ with Newton-Raphson iteration method.

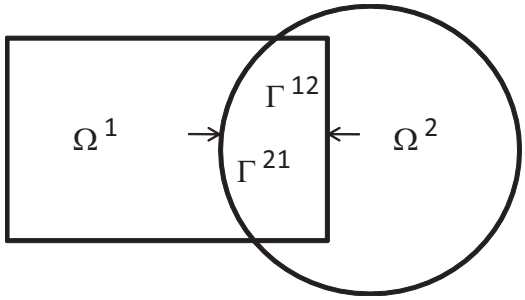


Figure 1. Domain decomposition for the case of two domains.

IV. Validation

Developed domain decomposition procedure was validated on a benchmark problem of a turbulent swept flow over a single wire in a channel, which is a simplified model of a realistic wire-wrapped fuel pin assembly first proposed by Ranjan et al.[6] and later investigated with a single-domain version of NEK5000 by Merzari et al.[7] The geometry consists of a channel with a wire embedded in one of the walls. Channel size is $4\pi\times2\times8\pi$ normalized by the channel half-width in x, y and z-directions, respectively, and the wire is a cylinder with the radius $R = 0.5$ in contact with the bottom wall (axis of symmetry is located at $x/h = 0$, $y/h = 0.5$, where h is the channel half-width). Two meshes used for simulations of a single wire configuration with the domain decomposition method are shown in Fig. 2. It consists of roughly 15000 elements, and polynomial functions of 6th through 9th order are used for spectral approximation within each element. Realistic wire-wrapped fuel pin assemblies are subject to a strong axial flow in the direction of the fuel pins and a weaker cross-flow due to the coolant-pin interaction. To model these effects, an axial bulk velocity W (in z direction) and a cross-flow bulk velocity $U/W = 1/6$ (in x direction) is imposed in the current configuration, with Reynolds number $Re_z = Wh/\nu = 6000$ to correspond to the simulations of Ranjan et al.[6] and Merzari et al.[7] All length scales are normalized with h, and velocities - with W in the current simulations. Mean flow rates are sustained in the simulations by imposing corresponding pressure gradients calculated dynamically through a feed-back control loop with periodic boundary conditions. Pressure gradient in a cross-flow direction is only applied to the exterior domain, while the interior domain is coupled to the exterior domain via interface conditions in a cross-flow direction. Axial pressure gradient is imposed in both domains.

To model heat transfer in the fuel pin assembly, a constant heat flux $q'' = 1$ is prescribed at the top and bottom walls of the channel (which represent the surfaces of the neighboring pins), while adiabatic boundary conditions (zero heat flux $q'' = 0$) are prescribed on the surface of the wire. It was shown in Ghaddar et al.[8] that the mean temperature grows linearly in the direction of a forced convection with the imposition of a prescribed flux on the surrounding surfaces. In the current configuration the direction of linear growth is the axial direction and one can write $T(\mathbf{x}, t) = \gamma\, z + \Theta(\mathbf{x}, t)$, with $\Theta(\mathbf{x}, t)$ periodic function in z. The growth coefficient γ is equal to

$$\gamma = \frac{\alpha\, q'}{k\, W\, Vol}, \tag{2}$$

where α is the thermal diffusivity, k is the thermal conductivity, $q' = \int_{\partial\Omega} q''\, d\, A$ is the total heat transfer rate into the domain, and Vol is the volume of the domain. Thus, periodic boundary conditions can now be used for $\Theta(\mathbf{x}, t)$ with the term $-w\,\gamma$ added as the source term to the energy equation (w is the local axial velocity). We take the coolant to be a liquid sodium, with high thermal conductivity resulting in a low Prandtl number $Pr = \nu/\alpha = 0.01$.

Instantaneous and time-averaged axial and crossflow velocities in a z-normal plane are shown in Figs. 3 and 4, respectively. Statistics were collected during the computational period $TW/h = 100$ Flow separation and reverse flow zone behind the wire is noticeable, consistent with the simulations.[6,7] Slight discontinuities in the axial velocity upstream of the sphere in the exterior domain are due to the relatively coarse grid resolution in x-direction in the sphere boundary layer. Axial velocity in the interior domain, with finer

resolution, is perfectly smooth. Axial velocity profiles are compared to the simulations of Ranjan et al.[6] and Merzari et al[7] in Fig. 5. Good agreement with both datasets is obtained.

Figure 10 shows the mean normalized temperature distribution $\overline{\Theta} = (\Theta - \Theta_{min})/(\Theta_{max} - \Theta_{min})$ in the coolant. Temperature distribution in the coolant above the line of contact ($x/h = 0$) is plotted in Fig. 7a. Temperature of the coolant is higher further away from the insulated wire, since the influence of the heated top surface becomes stronger. A hot spot is noticeable beneath the wire, at a line of contact of the wire with the pin wall, which occurs due to the slow heat removal at a stagnation region. Surface temperature along the x axis is plotted in Fig. 7b, clearly showing the effect of a hot spot. Agreement between the solutions in the two domains is excellent, showing that interface conditions work properly. In fact, maximum surface temperature is attained underneath the hot spot. To assess the effect of heat transfer due to the axial convection, crossflow convection and vertical conduction, it is useful to estimate the maximum temperature variation $\Delta\overline{T} = \Delta T/(\Theta_{max} - \Theta_{min})$ in vertical (above the contact line), crossflow (along the surface) and axial direction ($\Delta T_z = \gamma L_z$). Thus, the ratio of vertical/crossflow/axial temperature variation is $\Delta\overline{T}_y/\Delta\overline{T}_x/\Delta\overline{T}_z = 0.16/0.8/4.00 = 0.04/0.2/1$. It is seen that the axial temperature variation due to the forced convection is still dominant, and the heating effect due to a stagnation point flow is not crucial in the current configuration. The knowledge of the actual surface temperature in the vicinity of the hot spot is extremely important for the estimation of heat transfer characteristics of a particular assembly, but it becomes nearly impossible to estimate it for realistic fuel pin geometries (as discussed in the next section). This difficulty motivated the development of a domain decomposition method in the current code.

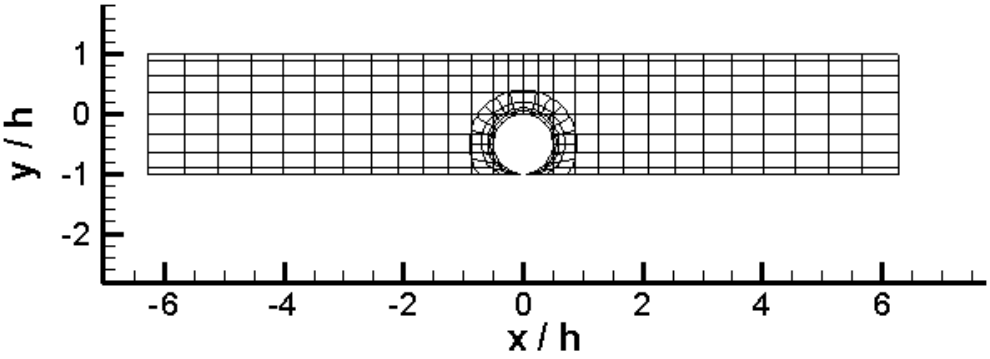
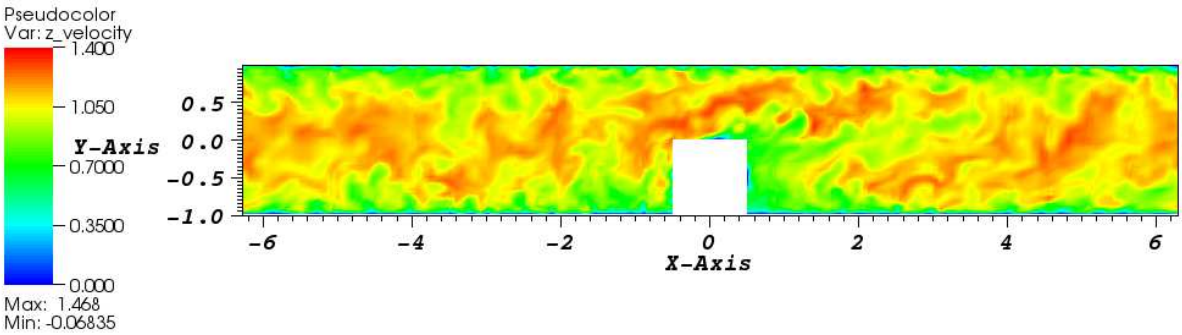


Figure 2. Overlapping meshes for the simulation of a single wire in a channel. Element boundaries are shown.

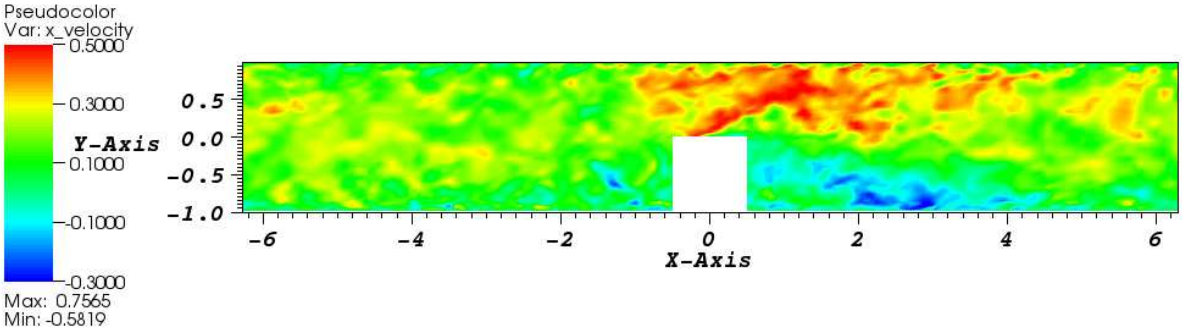
V. Wire-Wrapped Assemblies

Simulations of a fluid flow in actual fuel pin assemblies have been previously performed for 7-pin, 19-pin and full 217-pin configurations and hydrodynamics analysis of the flow has been documented.[2,3] Without recently developed domain decomposition capability, the fluid domain had to be discretized with a single hexahedral mesh. Numerical mesh used in the previously reported simulations is shown in Fig. 8. It is seen that in the framework of a single domain it is impossible to generate the mesh which would model exactly the shape of the wire and the pin in a place of their intersection: the intersection between the wire and the pin has to be smoothed out, and a singularity line where they intersect is not the part of the simulation. However it is the singularity line that is the likely place for the formation of a hot spot due to stagnation flow conditions. Thus, removing the singularity line and its vicinity from the model would severely jeopardize an accuracy of heat transfer prediction, and heat transfer analysis was not attempted in previously reported simulations.[2,3] In addition, approximating the fluid/solid interface by a smoothed line prohibits the development of a conjugate heat transfer simulations, since thermal boundary conditions on a physical fluid/solid boundary can not be provided.

In order to be able to address the question of the magnitude of heat fluxes at the intersection line between the pin and the wire, the calculations with two overlapping domains were initiated using the domain decomposition method implemented it NEK 5000 and described in the previous section. With the implementation of this method, in addition to being able to correctly represent the geometry at the intersection point, it



(a) Axial velocity



(b) Cross-flow velocity

Figure 3. Instantaneous velocity. Only exterior mesh is shown.

has also become possible to perform conjugate heat transfer study, solving for the coupled temperature field in the solid parts of the reactor (pin and wire wrap) and in the fluid parts (liquid metal coolant). The numerical mesh used in these calculations is shown in Fig. (9). Meshes for the two domains overlap in this figure: the inside domain contains the pin, the wire wrap and the thin layer of the fluid elements around the pin and the wire, and the outside mesh is the fluid mesh used in Ref. 2 (and shown in Fig. 8). Exchange of velocity and temperature variables is performed at every time step at the interface boundaries between the domains with the method described in the previous section. At this point, we model a single wire-wrapped pin, but extension to larger configurations (7-pin, 19-pin, 217-pin) are planned for the future. Preliminary results for the temperature inside the solid and the fluid domains obtained with the conjugate heat transfer simulations are displayed in Fig. 10.

VI. Conclusions

Domain decomposition method was developed and implemented in a spectral element Navier-Stokes solver NEK5000. The developed method was validated on a benchmark problem of a turbulent swept flow over a single wire in a channel. This development will enable a comprehensive study of heat transfer in realistic wire-wrapped fuel-pin assemblies designed for advanced burner reactors.

VII. Acknowledgements

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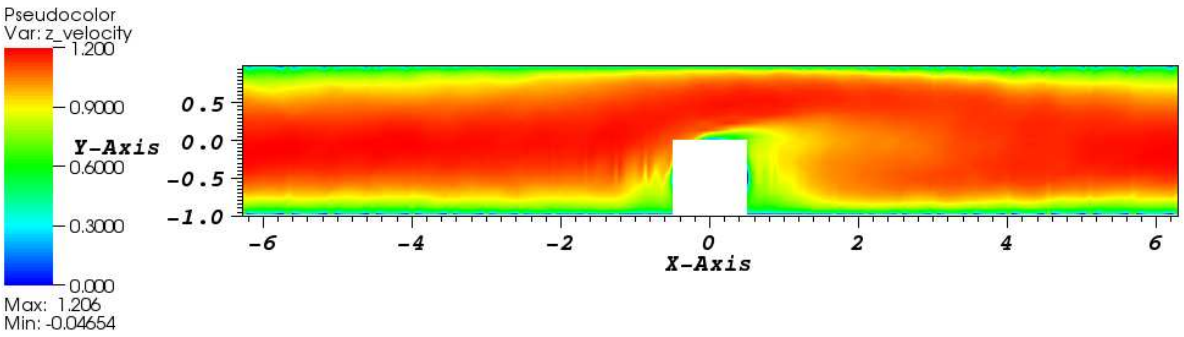
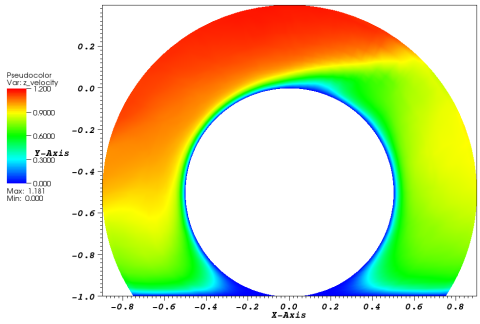
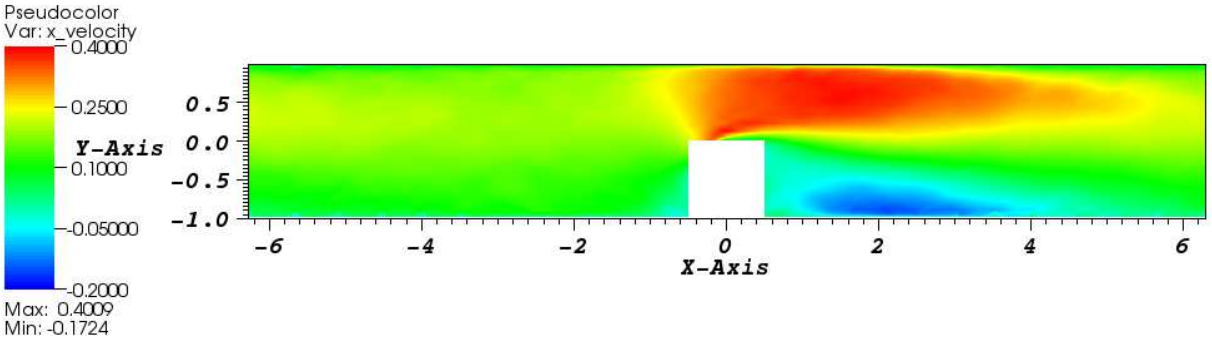


(a) Axial velocity. Exterior mesh.

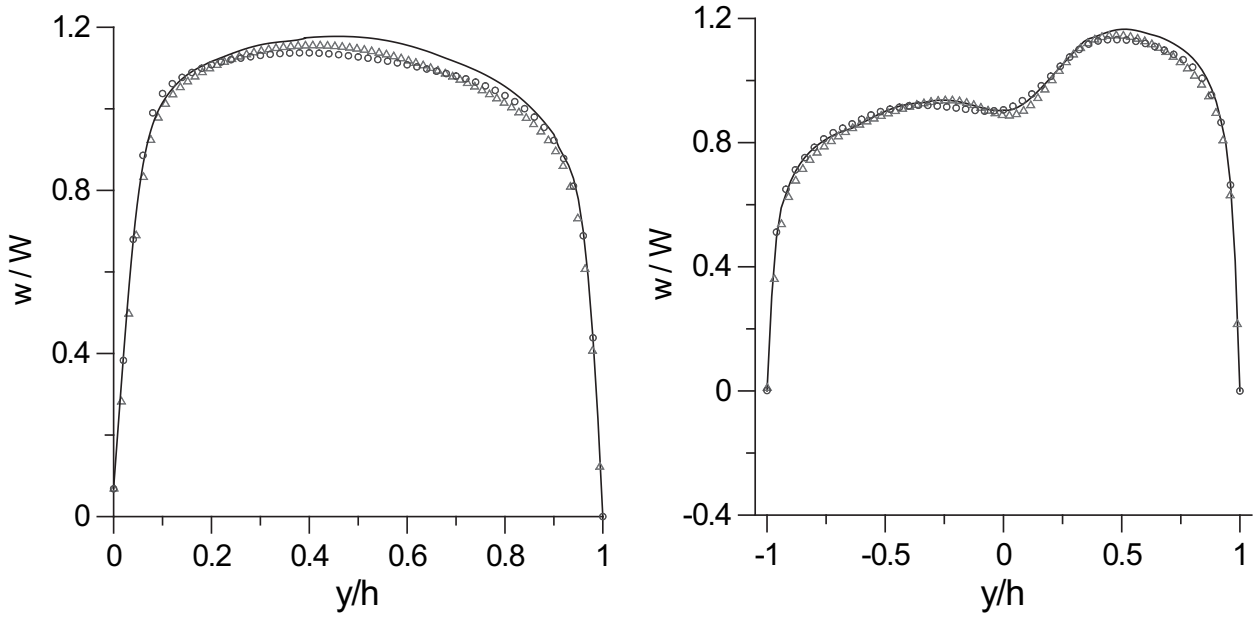


(b) Axial velocity. Interior mesh (enlarged).



(c) Cross-flow velocity. Exterior mesh.

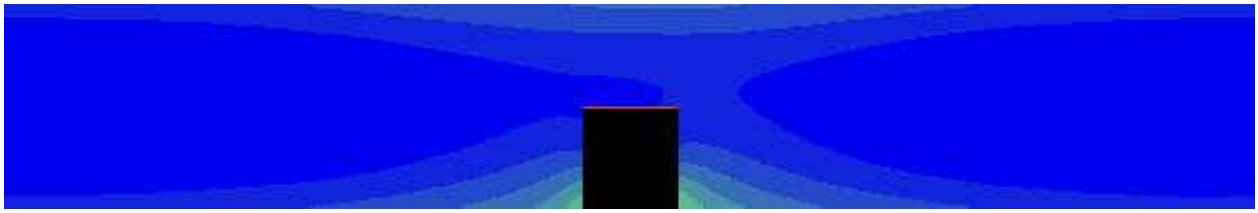
Figure 4. Mean velocity.



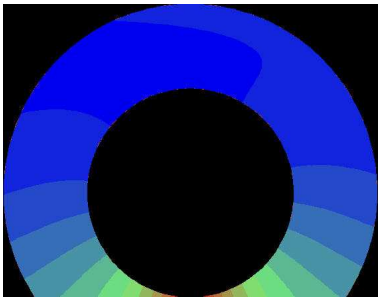
(a) $x/h = 0$ (wire centerline)

(b) $x/h = 1$

Figure 5. Comparison of axial velocity profiles with the other simulations. Solid line, current LES; triangles, DNS of Ranjan et al.;[6] circles, LES of Merzari et al.[7]

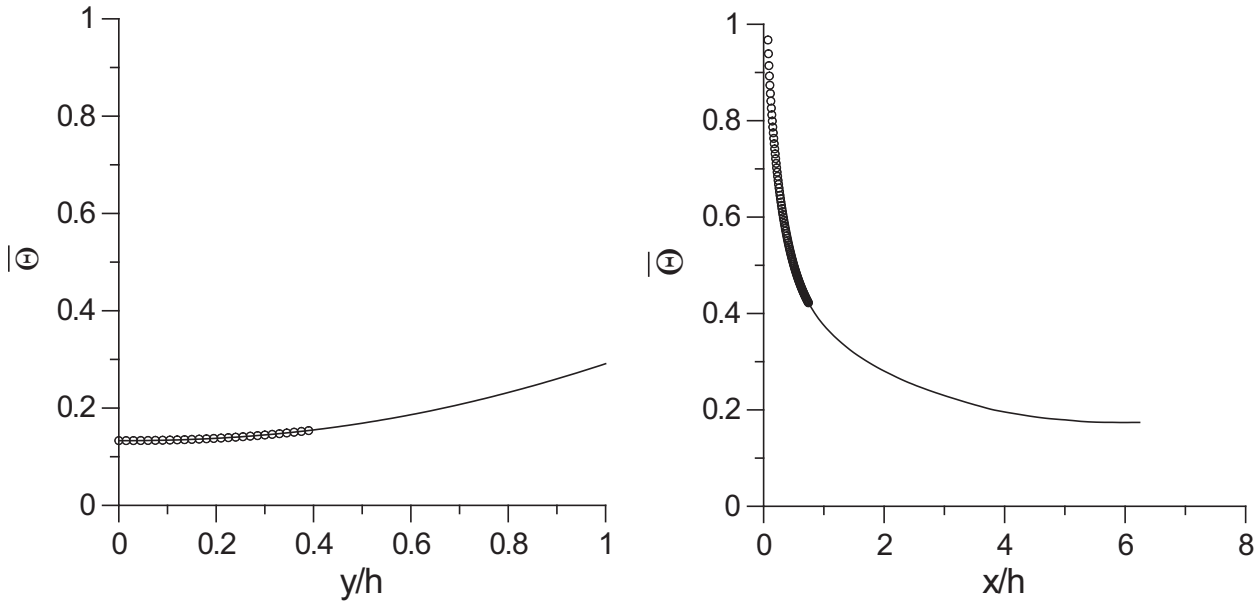


(a) Exterior mesh



(b) Interior mesh (enlarged)

Figure 6. Normalized temperature distribution in the channel. Blue color: value of 0; red color: value of 1.



(a) Across y axis, $x/h = 0$

(b) Across x axis, at the surface.

Figure 7. Temperature profiles. Symbols - interior mesh, solid line - exterior mesh.

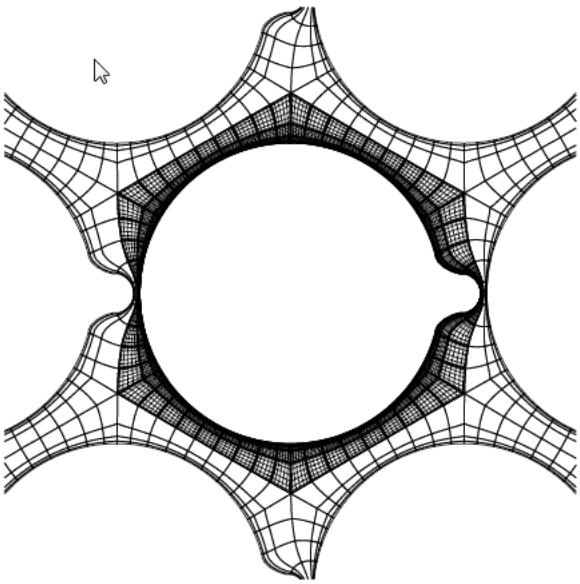


Figure 8. Numerical mesh used in the simulations of Ref. 2, 3.

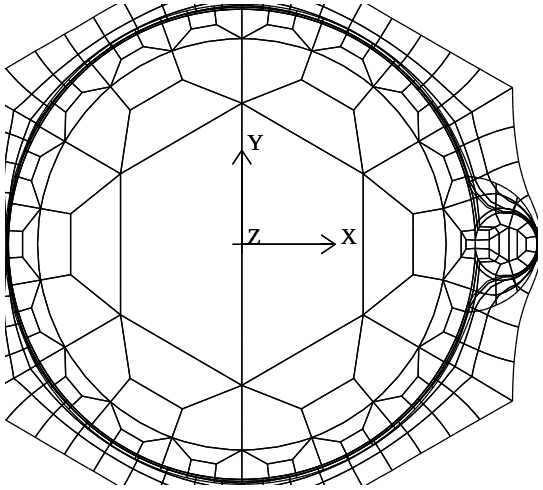


Figure 9. Numerical mesh used in the current conjugate heat transfer simulations with domain decomposition method.

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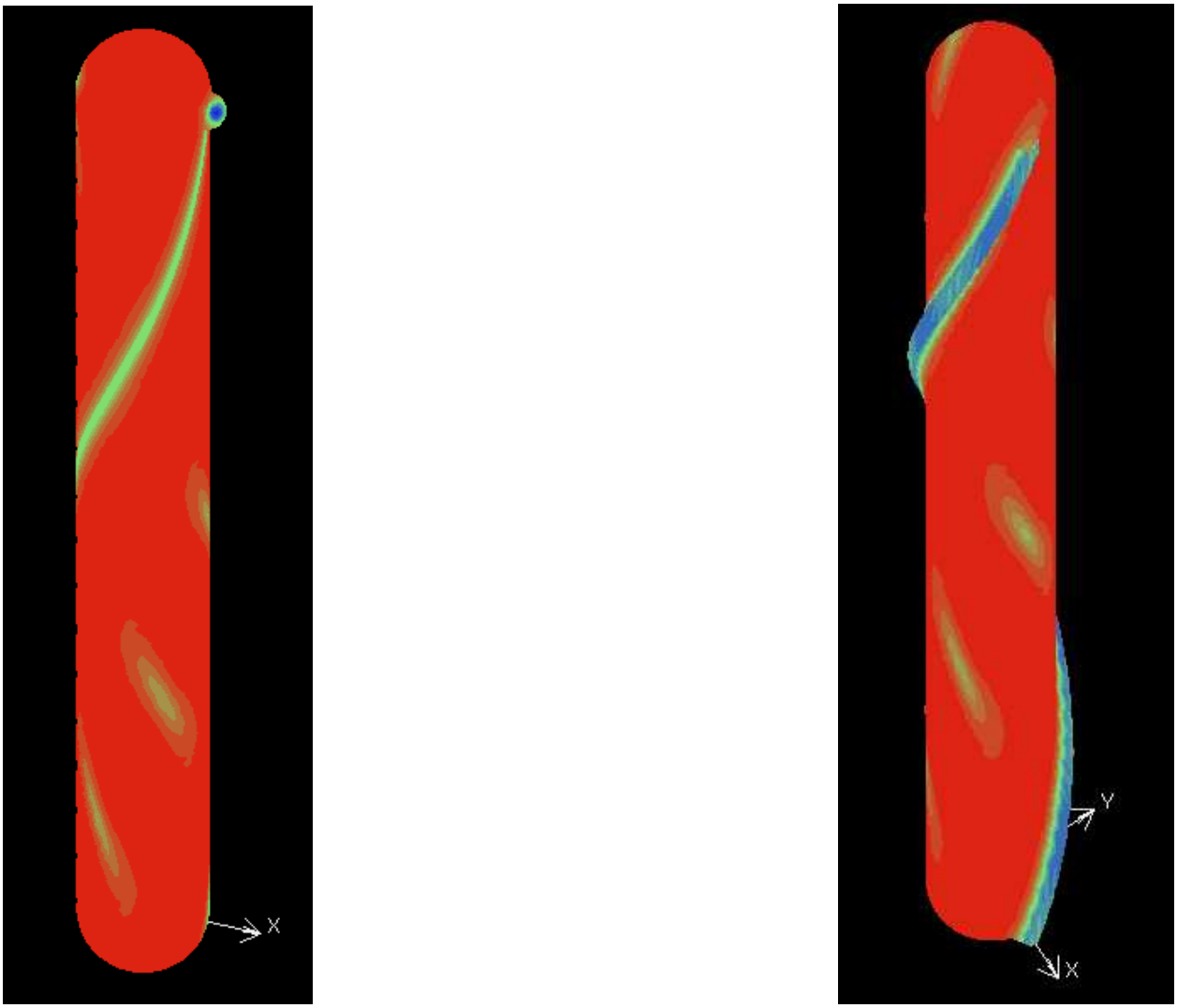

(a) Solid (inside domain)

(b) Fluid (outside domain)

Figure 10. Temperature distribution in the solid and the fluid