

Automated MATLAB®–COMSOL Generation of Solver-Ready Cerebrovascular Fluid–Structure Interaction Models

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Abstract

Manual set-up of patient-specific fluid–structure interaction (FSI) models remains a major bottleneck in cerebrovascular simulation, not only because meshing complex vascular anatomy is hard to automate, but because translating a mesh into a configured multiphysics solver model is itself an ad hoc, per-case task. We present an automated MATLAB®–COMSOL pipeline that closes this tooling gap end to end, converting cerebrovascular centreline data directly into solver-ready, structured FSI models without manual intervention at any stage. The pipeline extends the vascularmd O-grid hexahedral meshing framework to complex branching geometry, repurposing its outermost mesh layer as the vessel wall and using mesh connectivity to identify the fluid, wall, fluid–solid interface, and inlet/outlet boundaries automatically. Its central tooling contribution is a NASTRAN-tagging bridge that carries these selections into a COMSOL physics template through LiveLink™ for MATLAB® so that a single pre-configured template is instantiated automatically for every new mesh, with no COMSOL-side reconfiguration required. By automating both mesh generation and COMSOL model assembly within a single scriptable toolchain, this work turns FSI model preparation from a manual, per-case task into a batchable one, providing a validated route from cerebrovascular centreline data to solver-ready simulation suitable for generating the large-scale datasets required for surrogate modelling.

Keywords: fluid–structure interaction, cerebral haemodynamics, automated meshing, structured hexahedral mesh, LiveLink™ for MATLAB®, surrogate modelling.

Introduction

In cerebrovascular modelling, fluid–structure interaction (FSI) simulation couples deformation of the arterial wall with the surrounding blood flow, providing an accurate prediction of wall shear stress (WSS) [1, 2]. WSS has been implicated in the development of atherosclerosis and ischaemic stroke [3, 4]. Because WSS cannot be measured directly in the cerebral circulation at the resolution required, it must instead be inferred from numerical simulation performed on imaging-derived geometry [5].

The principal cost of assembling an FSI simulation lies not in the solver but in meshing the geometrically complex cerebral vasculature, together with the manual editing this conventionally requires. Structured hexahedral meshes are attractive because boundary-layer resolution can be prescribed systematically, which matters directly for WSS, a quantity known to be sensitive to near-wall refinement [6]. Such meshes are, however, considerably harder to generate automatically than tetrahedral meshes [7], since tetrahedral elements fill complex, branching geometry such as the cerebral arterial network without manual intervention. This trade-off explains why automated vascular pipelines have historically relied on tetrahedral discretisation, despite reported CFD comparisons on validation geometries showing that hexahedral meshes require six to ten times fewer cells, and more than an

order of magnitude less computational time, to reach a given accuracy than tetrahedral discretisations [8, 9]. Closing this gap between automatability and mesh quality is the central methodological challenge this work addresses.

Recent centreline-based methods have narrowed that gap. The vascularmd framework of Decroocq et al. [10, 11] constructs structured O-grid hexahedral meshes of vascular geometry directly from a centreline-and-radius description, without manual editing. Applied to 61 whole-brain networks from the BraVa database [12], it meshed 92 % of vessel segments and 83 % of bifurcations without producing invalid elements, demonstrating that structured meshing of complex cerebral geometry can indeed be automated. The meshes it produces, however, are intended for CFD analysis alone.

The gap this work addresses is consequently twofold. First, an FSI-ready mesh additionally requires a wall domain, a fluid–solid interface, and boundary sets that a solver can be directed to without manual selection, none of which follows from a CFD mesh. Block-structured hexahedral meshing has recently been extended to the FSI setting in its own right [13], but not from cerebral centreline databases, and not with automated identification of the domains and boundaries a multiphysics solver requires. Second, even given such a mesh, assembling it into a configured

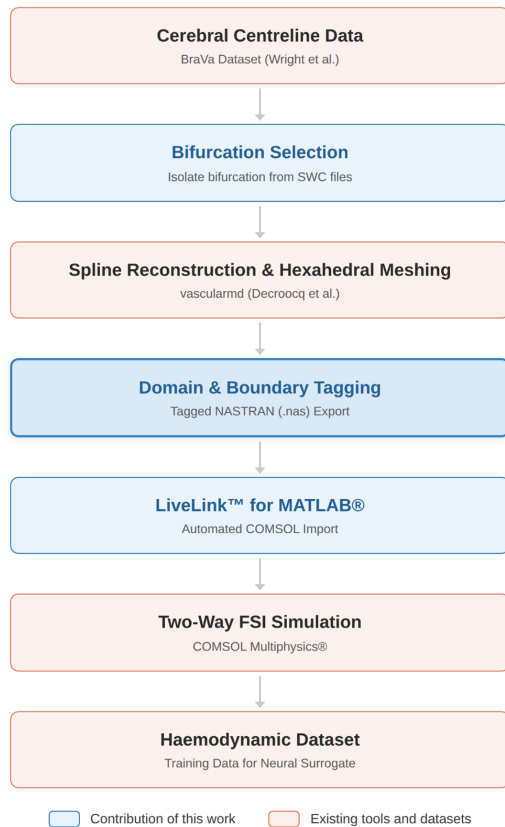


Figure 1. Structure of the automated pipeline, from BraVa centreline data to a batch of solver-ready COMSOL models. The automated meshing, tagging, and assembly stages contributed by this work are highlighted.

multiphysics model is ordinarily a manual operation. This is tolerable for a single simulation but prohibitive for the hundreds of simulations required to train a surrogate model, which is the longer-term motivation for the present work. The objective is therefore not to automate an individual simulation, but to automate the complete, reproducible transition from centreline data to a solver-ready FSI model.

We present an automated MATLAB®–COMSOL pipeline (Figure 1) that extends the centreline-based structured meshing method of Decroocq et al. [10] into a fully automated meshing methodology for complex FSI geometry. The contribution is threefold. First, the existing O-grid mesh topology is repurposed, with no additional manual geometry work, to define the vessel wall. Second, mesh connectivity alone is used to assign semantic domain and boundary tags automatically, without user interaction. Third, those tags are carried into COMSOL through NASTRAN and LiveLink™ for MATLAB®, allowing a single physics template to be reused automatically across every generated mesh. The pipeline is verified against an analytical solution for wave propagation in a fluid-filled elastic tube, and the sensitivity of predicted WSS to boundary-layer

mesh resolution is assessed across ten automatically generated meshes.

Methodology

Automated Pipeline

The central methodological contribution of this work is an automated meshing methodology that converts geometrically complex, patient-specific vascular geometry directly into a structured, solver-ready FSI mesh, with no manual intervention at any stage. The pipeline transforms a whole-brain centreline reconstruction into a batch of solver-ready FSI simulations in five stages: bifurcation selection, geometric modelling, structured hexahedral meshing, automated FSI tagging, and automated model assembly (Figure 1). Selection and assembly are implemented in MATLAB®; geometric modelling, meshing, and tagging are implemented in Python. Critically, no stage requires manual interaction with the geometry, which is what allows the pipeline to scale from a single simulation to the large batches needed for surrogate-model training.

Geometry Selection

The BraVa dataset provides centreline reconstructions of the cerebral vasculature of 61 healthy adults [12]. Each subject is represented as an .swc file organised as a tree, in which every node carries the coordinates (x, y, z) of the local vessel centreline, the local arterial radius r , and the identifier of its parent node, so that both branching points and segments of rapidly changing curvature are encoded explicitly. The whole-brain centreline reconstruction of a 24-year-old female subject, BG001.CNG.swc is loaded into MATLAB® and its 98 branching nodes are identified automatically. Only bifurcations with four nodes leading up to the branching node and four nodes in each daughter branch, with no further branching within that window, are retained: 65 of the 98 qualify, and each is written to a standalone .swc file so that only the corresponding local geometry is meshed, see Figure 2. The radii are then inflated by 5%, so that the exported centreline describes the outer wall surface and the wall thickness enters the pipeline as an explicit input parameter, one that is recovered exactly within the mesh through the cross-section layer ratios described below.

Automated Structured Hexahedral Meshing of Complex Vascular Geometry

Following Decroocq et al. [10], a smooth geometric approximation of the vessel is first constructed from the .swc centreline data. The volume mesh is then generated automatically and divided radially into three bands, with extents fixed as the fractions 16/21, 4/21, and 1/21 of the local outer radius, measured from the

core outwards [10]. Because the radii were inflated by 5% at the geometry-selection stage, the outermost band spans exactly the prescribed wall thickness. For the validation geometry of the following section (outer radius 2.1 mm), this reproduces the 0.1 mm benchmark wall thickness identically; for the bifurcation reconstructions, the fluid domain corresponds exactly to the local radius recorded in the original BG001.CNG.swc file. This repurposing of an existing CFD meshing topology, rather than the construction of a separate wall geometry, is what allows a solid wall domain to be generated automatically for arbitrarily complex branching geometry.

Mesh resolution is controlled by four parameters, all scriptable from MATLAB® and therefore automatable across an arbitrary batch of geometries: the number of circumferential nodes N , the axial ring spacing d , and the number of radial element layers through the wall ($n_a + 1$) and through the near-wall fluid band ($n_b + 1$) [10]. The baseline configuration is $N=24$, $d=0.32$, $n_a=1$, $n_b=3$. Every generated mesh is checked automatically for element quality: the scaled Jacobian of each cell is computed, and the pipeline asserts that no degenerate or inverted elements are present before the mesh proceeds to tagging.

Automated FSI Tagging

The mesh is exported in NASTRAN format, in which every element carries a property identifier (PID). All hexahedral (CHEXA) elements are first assigned PID 1, representing the fluid domain, as highlighted in Figure 2. A second pass, mirroring the logic of the mesh generator, reassigns the elements of the outermost cross-section band to PID 2, representing the wall; the two volumetric domains are thereby separated automatically, without reference to any manually selected geometry.

Boundary faces are then recovered from element connectivity alone, again without manual selection. A face shared by a PID-1 element and a PID-2 element is tagged as the fluid–solid interface; a PID-2 face with no neighbouring element on its outward side is tagged as the outer wall; and, on each end cap, faces belonging to PID-1 elements form the inlet or outlets, while faces belonging to PID-2 elements form the wall annulus. These faces are written as CQUAD4 shell elements carrying the tags listed in Table 1. Before export, the tagging is verified automatically: every selection is confirmed non-empty, and the number of connected components in the inlet, outlet, and annulus-cap selections is checked, so that a malformed mesh is rejected rather than silently propagated downstream.

On import, COMSOL converts CHEXA PIDs into domain selections and CQUAD4 PIDs into boundary selections automatically, so that the physics setup can address every region of the model by tag number rather than by manual picking. This is the mechanism by

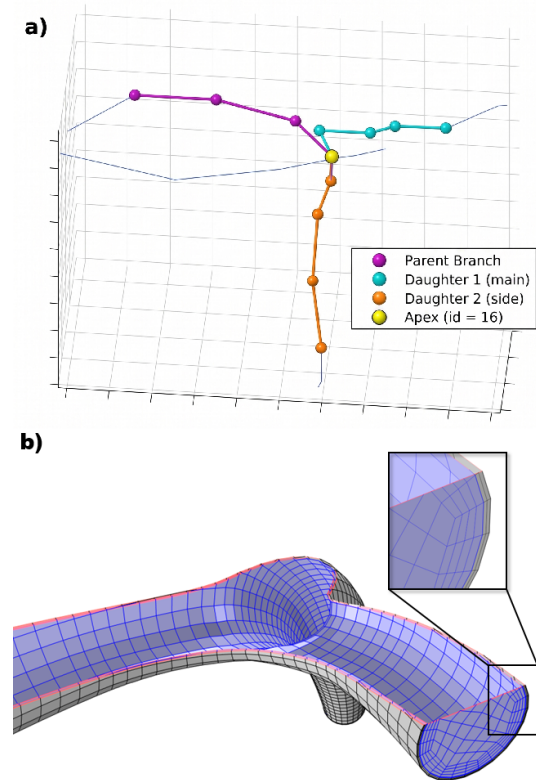


Figure 2. Bifurcation 16 of BraVa subject BG001.CNG.swc. (a) The centreline nodes retained by the four-node selection window — the apex and the parent and two daughter branches — against the surrounding network (faint), which is excluded. (b) The FSI-ready NASTRAN mesh generated from those nodes, with the automatically tagged fluid domain (PID 1) highlighted and the wall (PID 2) in grey. The inset shows the O-grid cross-section at the outlet cap, in which the outermost band forms the wall and its inner surface the fluid–solid interface.

Table 1: Domain and boundary tags carried by the NASTRAN mesh

Entity	Element type	Tag
Fluid domain	CHEXA	1
Wall domain	CHEXA	2
Fluid–solid interface	CQUAD4	101
Inlet	CQUAD4	111
Outlet(s)	CQUAD4	131
Outer wall	CQUAD4	201
Wall-end annulus	CQUAD4	221

which the automated meshing methodology upstream connects directly to a configured multiphysics model, without requiring geometry-specific intervention in COMSOL Multiphysics® itself.

Automated Model Assembly

The physics is configured once, in a template .mph file, and bound entirely to the tags in Table 1. LiveLink™

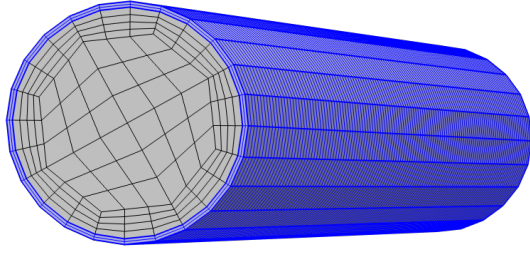


Figure 3. FSI-ready NASTRAN mesh, automatically tagged, with the solid domain highlighted. Reproducing the verification geometry of Liu and Fletcher [14].

for MATLAB® then instantiates this template automatically for each simulation: it connects to a COMSOL mphserver, repoints the NASTRAN import of the template at the new .nas file, and rebuilds the mesh. Because every selection is derived from the PIDs rather than from manually picked geometry, the entire physics setup survives this swap unchanged, and the resulting model is saved with the mesh embedded. One folder is built per simulation, and all simulations are zipped into a single archive ready for deployment on the HPC cluster. Because the physics and solver settings reside only in the template, generating a new simulation reduces entirely to generating a new automatically tagged NASTRAN mesh, which is the property that allows the pipeline to scale to the large batches required for surrogate-model training.

Verification

The pipeline is verified against the wave-propagation benchmark of Liu and Fletcher [14], in which a wave travels along a straight, fluid-filled elastic tube; all parameters are listed in Table 2. The geometry is generated through the same route as the bifurcation models described above: a straight centreline is passed to the automated meshing stage, and the resulting tagged NASTRAN mesh is imported into COMSOL without modification, see Figure 3. The verification therefore exercises the production pipeline directly, rather than a separately constructed model, and so tests the automated meshing methodology on the same terms as the cerebrovascular application.

Ten meshes were generated for the validation geometry, as listed in Table 4. Because the cross-section layer ratios are fixed, all ten discretise an identical geometry, including the same 0.1 mm wall, and differ only in resolution: circumferential (N), axial (d), through the wall (n_a), and through the near-wall fluid band (n_b).

The model couples the Laminar Flow and Solid Mechanics interfaces through the Fluid–Structure Interaction multiphysics coupling, with the fluid domain treated as a deforming domain under an arbitrary Lagrangian–Eulerian description.

The wall is modelled as a linear elastic material with geometric linearity, and the fluid as an incompressible

Table 2: Benchmark parameters, after Liu and Fletcher [14]

Quantity	Symbol	Value
Inner radius	R_i	2×10^{-3} m
Wall thickness	h	1×10^{-4} m
Tube length	L	80×10^{-3} m
Wall density	ρ_s	1000 kg m^{-3}
Young’s modulus	E	1×10^6 Pa
Poisson’s ratio	ν	0.4999
Fluid density	ρ	1000 kg m^{-3}
Dynamic viscosity	μ	1×10^{-3} Pa s
Pressure ramp rate	k	$35\,250 \text{ Pa s}^{-1}$

Newtonian fluid, following Liu and Fletcher [14]. A pressure boundary condition is applied at the inlet, ramped linearly as

$$p(0, t) = kt, \quad (1)$$

with the outlet held at 0 Pa. Mesh motion at the inlet and outlet is restricted to a prescribed zero normal mesh displacement, which allows those faces to deform within their own planes while preventing axial drift. The inner surface of the wall carries the fluid–structure interface and the no-slip boundary condition.

The problem is solved using a time-dependent study with strict time stepping (BDF) over 6 ms, with results output every 0.5 ms. Manual time stepping was also tested, with step sizes of 0.5 ms, 0.25 ms, 0.125 ms, and 0.0625 ms; because the predicted wave speed proved highly sensitive to the size of the initial time step, the solver’s strict time-stepping option was used instead.

Analytical solution

For a thin-walled tube, the Moens–Korteweg wave speed [15] is

$$c_0 = \sqrt{\frac{Eh}{2\rho R_i}}, \quad (2)$$

which, for the parameters of Table 2, gives $c_0 = 5.00 \text{ m s}^{-1}$. When zero axial displacement is additionally enforced, this becomes

$$c_2 = \frac{c_0}{\sqrt{1 - \nu^2}} = 5.77 \text{ m s}^{-1}. \quad (3)$$

The corresponding radial displacement at the inlet follows from Womersley’s solution [16] as

$$\delta_{r0}(t) = \frac{ktR_i^2(1 - \nu^2)}{Eh}, \quad (4)$$

reaching $6.35 \text{ } \mu\text{m}$ at 6 ms, or 0.32 % of the undeformed radius. The corresponding simulated values across all ten meshes, and their agreement with these analytical predictions are reported in the next section.

Table 3: End-to-end application of the pipeline to one BraVa subject (BG001.CNG.swc). Rates in the lower block are relative to the preceding stage. Times are wall clock on a single workstation.

Stage	Cases	Rate	Time
Bifurcations in network	98		
Meeting selection criterion	65	66 %	1.3 s
Meshed (vascularmd), & tagged	55	84.6 %	306 s
Imported to COMSOL®	55	100 %	109 s
Solver-ready models	55		8.5 min

Results

End-to-end Cerebrovascular Demonstration

The results of the automation study are summarised in Table 3. Of the 98 bifurcations in subject BG001 of the BraVa dataset, 65 met the isolated-bifurcation selection criterion described in the Methodology; the remaining 33 lay too close to a neighbouring branching to satisfy the four-node window and were not attempted. Of the 65 attempted, the automated meshing stage produced valid meshes, free of inverted cells, for 55, a success rate of 84.6 % that is comparable to the 83 % reported for bifurcations in the original fluid-domain-only study [10].

All 55 meshes were tagged, exported to NASTRAN, and imported into COMSOL Multiphysics® through the LiveLink™ for MATLAB® template swap without a single failure (100 %), with every domain and boundary selection of Table 1 non-empty in the assembled model. The complete sequence, from centreline file to a batch of solver-ready models packaged for the HPC cluster, took 8.5 min on a single workstation equipped with an Intel® Core™ Ultra 7 165H processor and 32 GB RAM, using MATLAB® R2023b and COMSOL Multiphysics® 6.2. Meshing and the inverted-cell check accounted for the largest share of that time, at 5.1 min (4.7 s per case), with model assembly requiring a further 1.9 s per case and requiring no manual intervention. The figure reported here is the time to assemble solver-ready models, not the time to obtain converged solutions.

Mesh Sensitivity

Table 4 summarises the three validation metrics across all ten meshes, and Figure 4 replicates Figure 5 from [14]. The simulated wave speed agrees with the analytical value c_2 to within 0.41 % for every mesh; nine of the ten lie in a narrow band 0.31 % to 0.40 % below theory, and only the refined-wall case ($n_a=3$) sits marginally above it (0.22 %). The inlet radial displacement at 6 ms is within 1.5 % of the analytical value for all meshes (0.97 % at baseline).

Wall shear stress behaves differently. It is insensitive to N , d , and n_a , changing by no more than 1.2 % in the peak value, but it varies strongly and monotonically with the near-wall fluid resolution n_b : from −19.1 % (peak) at $n_b=1$ to 11.9 % at $n_b=15$, relative to the

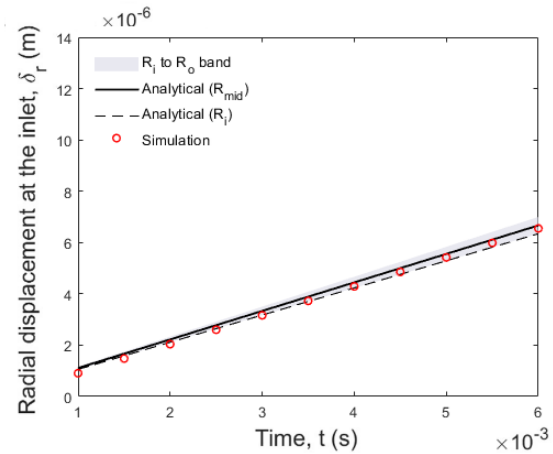


Figure 4. Radial displacement at the inlet as a function of time, reproducing the verification of Liu and Fletcher [14], compared with Eq. 4 evaluated at the mid-wall radius (solid) and at the inner radius (dashed); the shaded band spans R_i to R_o . The simulation lies within the band throughout, so the residual difference is smaller than the ambiguity in which radius the thin-wall solution refers to.

baseline. A change of approximately 3 % remains between $n_b=7$ and $n_b=15$, indicating that WSS is not yet fully mesh-independent even at the finest near-wall resolution tested.

Discussion

Assembling 55 solver-ready bifurcation models in under nine minutes, without manual intervention, removes the per-case CAD editing that otherwise sets the pace of dataset generation. Two observations support the specific design choices underlying the automated meshing methodology. First, inflating the centreline radii to carry the wall did not measurably degrade the meshing success rate relative to the fluid-domain-only method: 84.6 % here, against the 83 % reported by Decroocq et al. [10]. The two figures are not strictly comparable, since this is a single subject and the bifurcations are meshed in isolation rather than as a connected network, but the absence of any decline indicates that the wall domain is obtained essentially for free from the existing O-grid topology, without a dedicated wall-meshing step. Second, every assembled model carried non-empty selections for all seven tags of Table 1, so recovering the fluid–solid interface, the free wall, and the end faces from mesh connectivity alone is robust across geometrically distinct bifurcations, not only for the validation tube.

The validation study shows that mesh-resolution requirements are quantity-dependent. Wave speed and wall displacement are captured to within 0.4 % and 1.5 % on the coarsest meshes considered, which verifies the geometry, the material description, and the fluid–structure coupling produced by the automated pipeline. Wall shear stress is not converged over the

Table 4: Mesh parameter study and validation metrics. The first row is the baseline; the parameter varied in each subsequent case is set in bold. The wall contains n_a+1 element layers, and the near-wall fluid band contains n_b+1 ; d is the longitudinal ring spacing as a proportion of the local radius. Wave speed c is compared with the axially constrained analytical value $c_2 = 5.7731 \text{ m s}^{-1}$; the inlet radial displacement δ_{r0} at $t = 6 \text{ ms}$ is compared with the analytical value $6.346 \mu\text{m}$; and peak ($\tau_{\max}$) wall shear stress on the fluid–wall interface is compared against the baseline mesh.

N	d	n_a	n_b	Hexahedra	$c \text{ (m s}^{-1}\text{)}$	$\Delta c_2 \text{ (\%)}$	$\delta_{r0} \text{ (}\mu\text{m)}$	$\Delta \delta_{r0} \text{ (\%)}$	$\tau_{\max} \text{ (Pa)}$	$\Delta \tau_{\max} \text{ (\%)}$
24	0.32	1	3	21 600	5.7522	−0.36	6.407	0.97	0.5807	0.00
16	0.32	1	3	13 440	5.7542	−0.33	6.326	−0.32	0.5823	0.27
32	0.32	1	3	30 720	5.7519	−0.37	6.439	1.46	0.5799	−0.13
24	0.22	1	3	31 320	5.7519	−0.37	6.407	0.97	0.5836	0.51
24	0.48	1	3	14 400	5.7525	−0.36	6.407	0.97	0.5736	−1.22
24	0.32	0	3	18 720	5.7533	−0.34	6.409	1.00	0.5806	−0.01
24	0.32	3	3	27 360	5.7856	0.22	6.407	0.96	0.5807	0.01
24	0.32	1	1	15 840	5.7498	−0.40	6.408	0.97	0.4697	−19.11
24	0.32	1	7	33 120	5.7542	−0.33	6.407	0.97	0.6308	8.64
24	0.32	1	15	56 160	5.7550	−0.31	6.407	0.96	0.6499	11.92

same range: the residual 3 % change between $n_b=7$ and $n_b=15$ leaves the baseline mesh short of mesh independence for this quantity. Because WSS is the quantity of clinical interest, a WSS-targeted study must refine the near-wall fluid band specifically, rather than the mesh globally.

That requirement exposes a limitation of reusing the outermost O-grid band as the wall, illustrated in Figure 2: the same structured topology that makes the wall available automatically also ties its resolution to that of the fluid mesh. A graded near-wall fluid distribution, with a bias factor concentrating elements at the fluid–solid interface, would better resolve the WSS gradient without a comparable increase in wall resolution. The wall itself required only a single element layer through its thickness for both displacement and wave speed to reach grid independence, so this refinement need not be reciprocated in the solid domain.

Taken together, the results demonstrate that automated structured hexahedral meshing, connectivity-based FSI tagging, and template-driven COMSOL Multiphysics® model assembly compose into a single automated methodology that removes the preprocessing bottleneck in generating FSI training data from complex cerebral centreline geometry.

Conclusion

We have presented an automated meshing methodology, implemented as a MATLAB®–COMSOL pipeline, that converts centreline-derived cerebrovascular geometry directly into solver-ready structured FSI models, without manual domain or boundary selection at any stage. Applied to a single BraVa subject, 55 of 65 eligible bifurcations were converted into solver-ready models in 8.5 min, demonstrating that the costly manual preprocessing and model-assembly stage that otherwise limits FSI dataset generation is

largely eliminated. Analytical verification against an elastic-tube benchmark showed errors below 0.41 % in wave speed and 1.5 % in radial displacement across all ten meshes tested, confirming that the automated meshing methodology preserves solution accuracy for the bulk FSI response. The mesh sensitivity study further shows that wall shear stress requires substantially stronger near-wall refinement than these bulk quantities, a distinction the pipeline’s scriptable mesh-resolution parameters make straightforward to address. Together, these results establish a practical, fully automated route from complex cerebrovascular centreline data to solver-ready FSI simulation, suitable for generating the large-scale simulation datasets required for surrogate modelling, where manual preprocessing and model construction would otherwise be prohibitive.

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Code Availability

The MATLAB® and Python scripts used for automated vascular meshing, FSI tagging, and COMSOL model assembly are available at https://github.com/LexXxik/automated_network. The repository provides the implementation of the automated pipeline described in this work.

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