Physically Preconditioned HPC-Enabled Fluid-Structure Interaction Modeling with Novel Coupling Scheme

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GENERAL MOTIVATION

In combination with experimental data collection, the AneuX project investigates phenomenological and mechanistic modelling to assess aneurysm disease progression, rupture risk, and the impact of various treatment options. Fluid-Structure Interaction (FSI) modelling provides information about (peak/cyclic/gradient/…) pressure and shear stress that is required as part of the mechano-transduction pathway model.

This requires functionality for image-based geometry creation, discretization, FSI simulation, and analysis. The FSI simulator must support complex, incompressible, nonlinear tissue models and needs to provide the necessary accuracy, scalability, and speed. For that purpose, novel coupling and preconditioning schemes have been developed.

PLATFORM

a. Sim4Life

Sim4Life [1] is a simulation platform for computational life sciences that is centered around high-resolution, detailed anatomical models functionalized with dynamic physiology and tissue models. The platform features image-based modelling (Fig. 1), HPC-enabled solvers, a modular GUI, VTK and OpenGL-based visualization, a Python scripting interface, and a pipeline framework for advanced analysis.

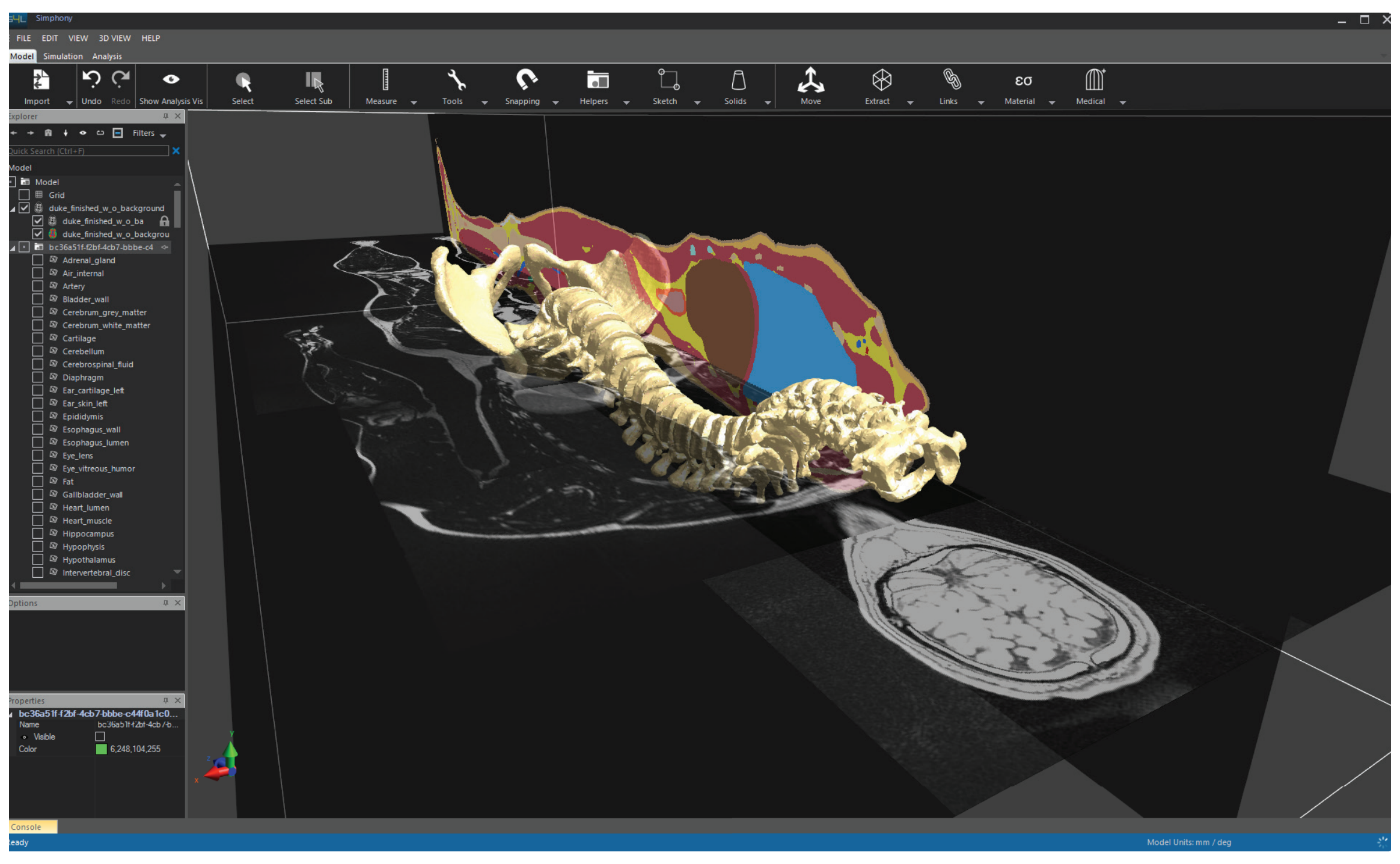

Figure 1 : *The Sim4Life platform is optimized for computational life sciences applications involving the human body and image-based modeling.*

b. Solver framework

A PETSc-based [2] FEM solver framework that enables the rapid generation of novel HPC-enabled solvers has been developed. It handles mixed-element meshes (tetrahedrons, prisms, hexahedrons, pyramids, etc.), flexible boundary conditions, file-I/O, and communication with Sim4Life. The framework supports a wide range of platforms (desktop, clusters, supercomputers) and parallelization paradigms (MPI, GPU, and pthread).

c. Vascular geometry generation

A novel image segmentation technique, which depends on line-shaped profiles [3] to allow generation of likelihood maps based on each pixel's neighborhood, has been developed to construct personalized vascular models. An interactive component in the form of the differential image foresting transform [4] that allows on-the-fly correction and segmentation of additional vessel segments has been added. It has been successfully applied to MRA and CTA images, validated against ground truth data, and is not restricted to healthy, tubular vessels. Surface extraction functionality that features volume preserving smoothing, element quality optimization, and mesh simplification has been developed. Furthermore, tools to extract centerlines, radii, and topologies of vascular trees [5] are integrated.

d. 1D FSI model

To model realistic flow conditions within the complete vascular network, coupling of the 3D FSI simulations with a pseudo-1D vascular trees model [6] simulating vascular flow in compliant (elastic or viscoelastic) vascular trees has been implemented - thus providing realistic boundary conditions and reducing the 3D computational domain - and verified using the method of manufactured solutions.

NOVEL NUMERICAL METHODS FOR FSI

a. FSI methods coupling scheme

The simulation of FSI involves solving three problems: fluid dynamics, solid mechanics, and fluid domain displacement. Three algorithmic approaches are widely applied: Monolithic, Semi-Implicit, and Partitioned (Fig. 3).

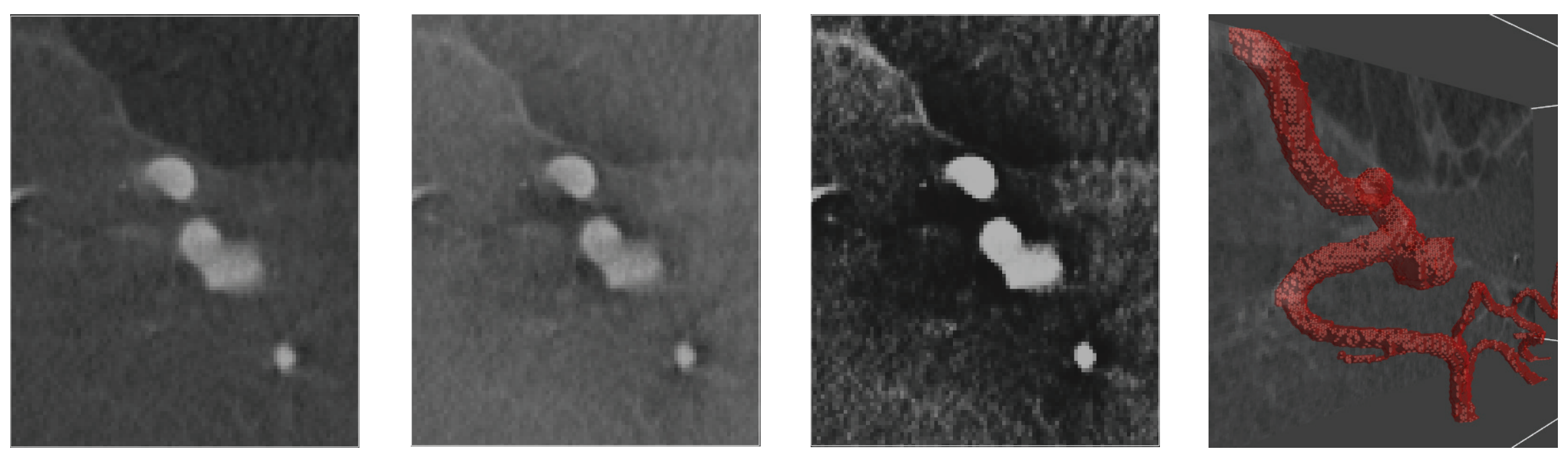

Figure 2: *The different stages of the segmentation process: (f.l.t.r) original image; result after processing with line-shaped profiles; likelihood map after applying a sigmoid; segmentation obtained by the image foresting transform before surface processing.*

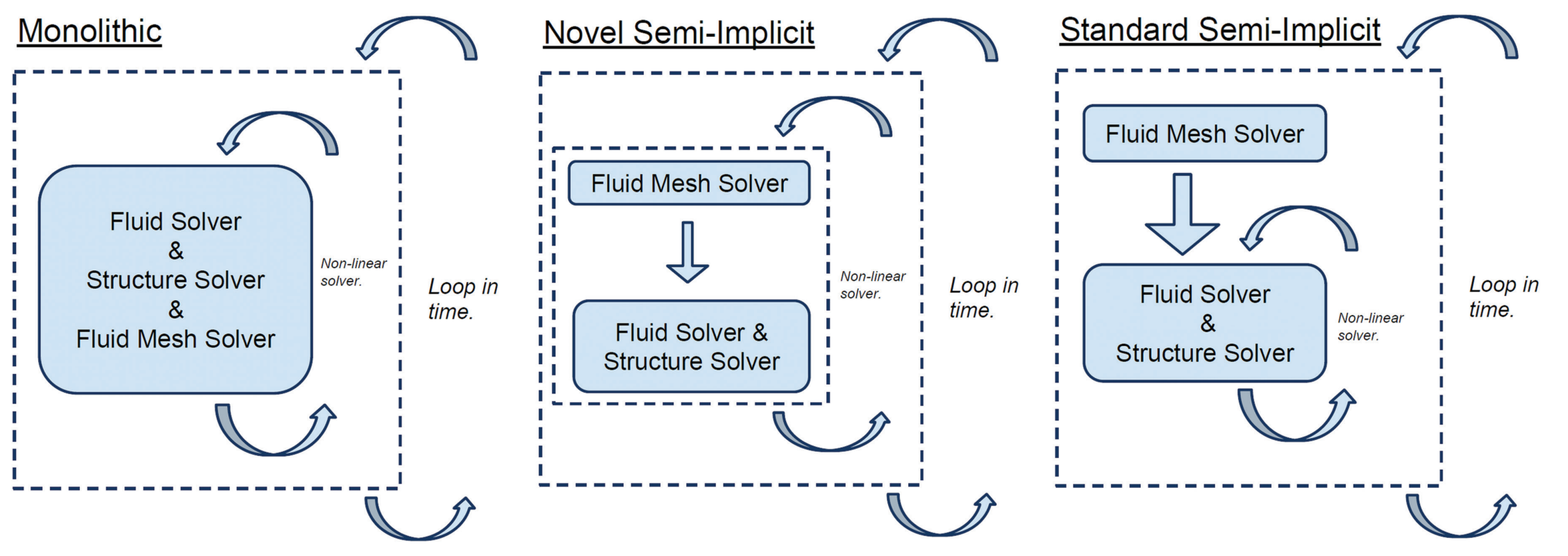

Figure 3 : *Schematic representation of different coupling approaches.*

The partitioned approach offers lower computational cost and accuracy, but is not suitable for biomedical applications due to the similarity of the fluid and solid densities. The monolithic approach is very robust and accurate even for biomedical applications, but computationally expensive. The semi-implicit approach, in which accuracy and computational effort are balanced, reduces the solving time, but can also degrade fluid domain element quality at the interface, as the solid moves while the fluid domain remains static, awaiting its own update. To overcome the drawbacks of the semi-implicit approach, a novel variant is presented, whereby the system is decomposed at the nonlinear iteration level, instead of at the time discretization level [7]. Monolithic robustness is retained because all variables are jointly updated, and computational complexity is reduced as the fluid mesh displacement can be highly optimized. In Figure 3, the standard methods are compared with the novel approach. All of these methods have been implemented in the solver framework and validated by means of the method of manufactured solutions, featuring elements of the Womersley theory of flow through elastic tubes [8].

The performance of the new approach in comparison to conventional ones was investigated by simulating fluid flow through a tube with a flexible wall (Newtonian fluid, density: 1000 kg/m^3, dynamic viscosity: 0.001 Pa·s, Reynolds number: 1000; St. Venant-Kirchhoff law, Young modulus: 0.1 MPa, Poisson ratio: 0.33; linear solver: MUMPS, Newton Method with Line Search). The results in Table 1 demonstrate the reduced computational cost.

Coupling scheme	Size of the strongly coupled system [#DOF]	Size of the fluid domain system [#DOF]	Avg. number of Newton iterations / time-step	Avg. time per time-step [s]
Monolithic	15622	-	3.81	48.8
Novel S.I	11707	3915	2.0	6.88
Standard S.I.	11707	3915	3.58	7.77

Table 1: *Comparison of computational performance and cost for the different coupling schemes. The novel semi-implicit approach combines the advantages of the monolithic and standard semi-implicit methods and even results in a lower number of Newton iterations.*

b. Physically based preconditioners

To further enhance convergence and performance, a multi-level physically-motivated preconditioning approach was devised. It starts by employing Schur factorization to solve the Fluid-Structure sub-block. In matrix form, this reads:

$$A_{fsi} = \begin{bmatrix} A_s & A_{force} \\ A_{vel} & A_f \end{bmatrix}$$

where A_s, A_f, A_{vel}, A_{force} are the Jacobians of the solid, fluid, kinematic, and dynamic compatibility conditions, respectively. A_f is itself a block matrix:

$$A_f = \begin{bmatrix} A_{vv} & A_{vp} \\ A_{pv} & A_{pp} \end{bmatrix}$$

where A_{vv} and A_{pp} relate to velocity and pressure, respectively. The Schur factorization aproximates the inverse as

$$A_{fsi}^{-1} = \begin{bmatrix} A_s^{-1} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & -A_{force} \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & S_{fsi}^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -A_{vel}\, A_s^{-1} & I \end{bmatrix}$$

The Schur complement $S_{fsi} = A_f - A_{vel} A_s^{-1} A_{force}$ is given by

$$S_{fsi} = \begin{bmatrix} A_{vv} - A_{vel} A_s^{-1} A_{for,v} & A_{vp} - A_{vel} A_s^{-1} A_{for,p} \\ A_{pv} & A_{pp} \end{bmatrix} = \begin{bmatrix} B_{vv} & B_{vp} \\ A_{pv} & A_{pp} \end{bmatrix}$$

and is actually the Fluid momentum equation "disturbed" at the interface entries. Schur factorization is applied again at the level of S_{fsi} and already established preconditioners can then be used:

$$S_{fsi}^{-1} = \begin{bmatrix} B_{vv}^{-1} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & -B_{vp} \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & S_f^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -A_{pv}\, B_{vv}^{-1} & I \end{bmatrix}$$

where the second level Schur complement S_f is

$$S_f = A_{pp} - A_{pv}\, B_{vv}^{-1}\, B_{vp}$$

For incompressible mechanical materials, the Schur factorization is also applied to the block A_s. The solving of every subsystem benefits from the wide range of linear solvers available within PETSc, and global preconditioning is achieved by a fixed number of KSP iterations [9]. Currently, a thorough study of the efficiency of the novel preconditioning approach is being conducted.

CONCLUSIONS

A novel semi-implicit FSI approach that retains the low computational cost while achieving monolithic accuracy has been developed, implemented within a HPC framework, and validated. A physically-motivated multi-level preconditioning approach has been developed to further boost performance. The solver already supports incompressible non-linear material models (Neo-Hookean and Mooney-Rivlin) and is embedded in a comprehensive computational life sciences platform that also features novel image-based vasculature generation functionality for personalized modeling. Further optimization of solver performance, extension of the supported constitutive material laws to encompass fiber-enforced behavior relevant for vessel wall modeling, and coupling of the FSI modeling to Windkessel elements and 1D vessel networks are ongoing, along with the implementation of the Variational Multiscale Stabilization method for both the fluid and the structure equations.

ACKNOWLEDGMENTS

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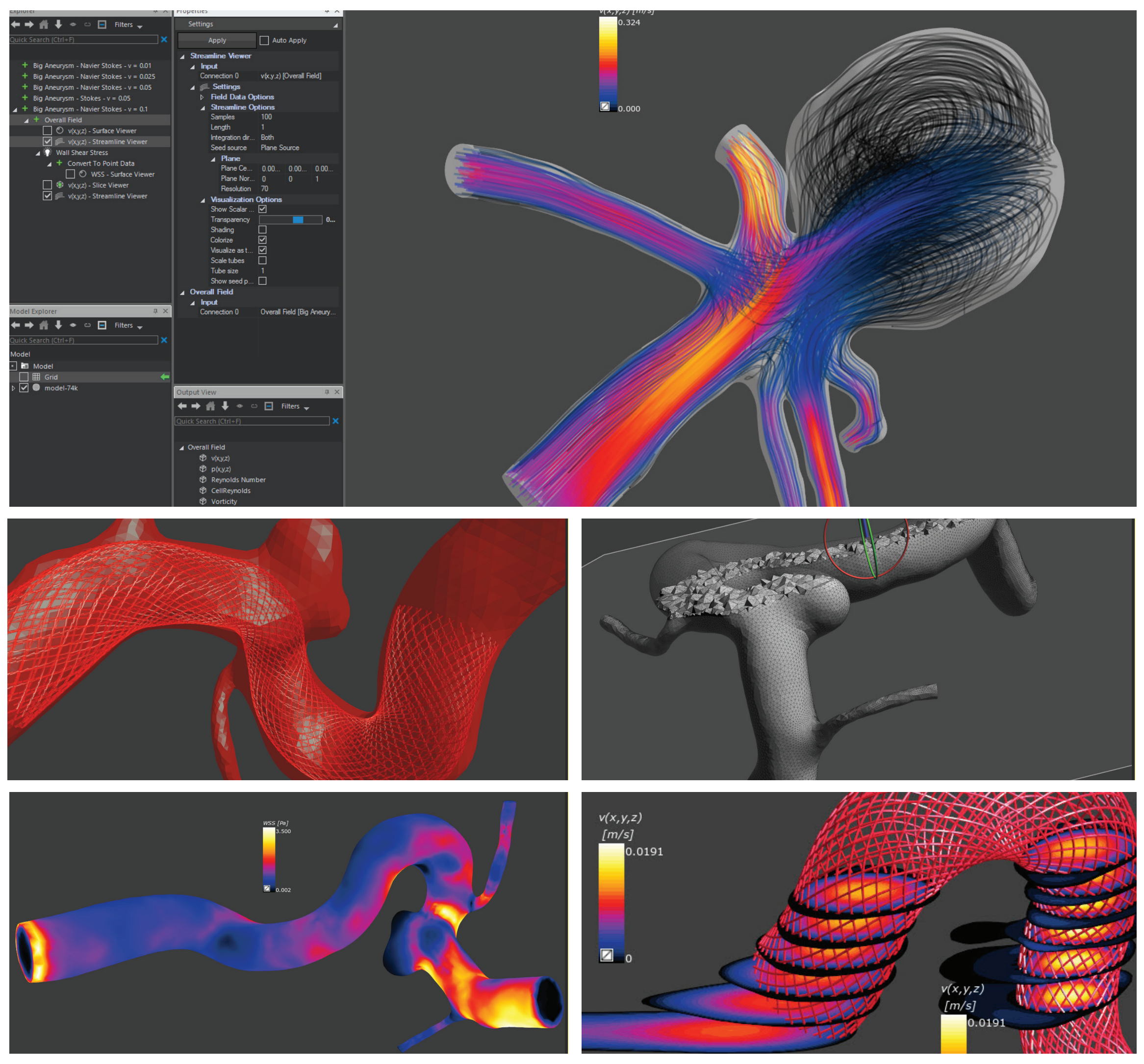

Figure 5: *Modeling of image-based treated (flow diverter) and untreated aneurysms. The visualizations show flow, velocity and wall shear-stress distributions.*

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