S.I. Residual-Based Variational Multiscale Formulation for Navier-Stokes-Brinkman Equations on moving domains

The Navier-Stokes-Brinkman (NSB) equations, originating from porous media theory, can be employed with the purpose of simulating viscous flow including complex shaped solid obstacles in a fluid domain, see \[S2\] and \[S1 \ S11\] for a in-depth mathematical analysis. The NSB model was successfully extended to moving obstacles and applied to model flapping insect flight in \[S13\]. In the present work, we use the NSB equations including the adaptation for moving obstacles as well as moving domains using the arbitrary lagrangian Eulerian (ALE) formulation \[S20 \ S22 \ S41\]:

\[
\begin{align*}
\rho \left( \frac{\partial}{\partial t} u + (u - w) \cdot \nabla u \right) - \nabla \cdot (\sigma(u, p) + \frac{\mu}{K} (u - u_s)) &= 0 & \text{in } \mathbb{R}^+ \times \Omega(t), \\
\nabla \cdot u &= 0 & \text{in } \mathbb{R}^+ \times \Omega(t), \\
u &= w & \text{on } \Gamma_{\text{noslip}}(t), \\
\sigma n - \rho \beta ((u - w) \cdot n) &= h & \text{on } \Gamma_{\text{outflow}}(t), \\
u &= g & \text{on } \Gamma_{\text{inflow}}(t), \\
u|_{t=0} &= u_0, \\
\end{align*}
\]

with the time dependent fluid domain \(\Omega(t)\) defined as

\[
\Omega(t) := \{ x \mid x = X + d(X, t), \forall X \in \Omega_0 \},
\]

using the ALE mapping \(d\) transforming an arbitrary reference configuration \(\Omega_0\) into the current fluid domain \(\Omega(t)\). Here \(p, u,\) and \(w := \frac{\partial}{\partial t} d\) represent the fluid pressure, the flow velocity, and the ALE velocity respectively, \(\mu\) is the dynamic viscosity and \(\rho\) the density. The volume penalization term \(\frac{\mu}{K(t, x)} (u(t, x) - u_s(t, x))\) is commonly known as Darcy drag which is characterized by the permeability \(K(t, x)\). Another interpretation of the Darcy drag can be given as resistance term, as for example aerodynamic drag is also interpreted as a resistance. In \[1\] the Darcy drag is modified to enforce correct no-slip conditions for obstacles moving with the obstacle velocity \(u_s(x, t)\). The fluid stress tensor \(\sigma(u, p)\) and strain rate tensor \(\epsilon(u, p)\) are defined as follows:

\[
\begin{align*}
\sigma(u, p) &= -\rho I + 2\mu \epsilon(u, p), & (7) \\
\epsilon(u, p) &= \frac{1}{2} (\nabla u + (\nabla u)^\top). & (8)
\end{align*}
\]
For \( h = 0 \), (3) is known as a directional do-nothing boundary condition \([S7][S32]\), where \( n \) is the outward normal of the fluid domain, \( \beta \leq \frac{1}{2} \) is a positive constant and (9) is added for backflow stabilization with
\[
((u - w) \cdot n)_- := \frac{1}{2}((u - w) \cdot n - |(u - w) \cdot n|).
\]

The ALE domain \( \Omega(t) \) is split up into three time dependent sub-domains by means of the permeability \( K(t, x) \), namely the fluid sub-domain \( \Omega_f(t) \), the porous sub-domain \( \Omega_p(t) \) and the solid sub-domain \( \Omega_s(t) \).

\[
K(t, x) = \begin{cases} 
K_f & \text{if } x \in \Omega_f(t) \\
K_p & \text{if } x \in \Omega_p(t) \\
K_s & \text{if } x \in \Omega_s(t)
\end{cases}
\]

In \( \Omega_f(t) \) the classical ALE-Navier–Stokes equations are recovered, while in \( \Omega_p \) the full ALE-NSB equations describe fluid flowing through a moving porous medium, \( u \) and \( p \) are understood in an averaged sense in this context. In \( \Omega_s(t) \) the velocity \( u \) is approaching \( u_s \) and thus asymptotically satisfying the no-slip condition on the \( \Omega_f(t)/\Omega_s(t) \) interface. Note that even in the case where \( K \to 0^+ \) the penalization term has a well-defined limit, see \([S1]\).

### S.I.A. Hemodynamic Afterload Models

Modeling of afterload for hemodynamics is modeled by using a 0D Windkessel model. This means we define \( h \) in (4) as
\[
h := -p_{WK}(t)n
\]
with the Windkessel pressure \( p_{WK} \) is governed by the differential algebraic system \([S76]\)
\[
C_{WK} \frac{d}{dt} p_d(t) + \frac{p_d(t)}{R_{WK}} = Q(t),
\]
\[
p_{WK}(t) = Z_{WK} Q(t) + p_d(t),
\]
\[
Q(t) := \int_{\Gamma_{\text{outflow}}} u \cdot n \, ds_x.
\]

In the case of multiple Windkessel outlets we will use the same notation for variables with an added \( i \) subscript indicating multiple outlets. Tools for personalization of the individual Windkessel parameters can be found in \([S33]\).

### S.I.B. Variational Formulation and Numerical Stabilization

Following \([S7][S8]\) the discrete variational formulation of (1) including the boundary conditions (4), (5) and (5) can be stated in the following abstract form: Find \( u^h \in [S^1_{h,0,ID}(\mathcal{T}_h)]^3 \), \( p^h \in S^1(\mathcal{T}_h) \) such that, for all \( v^h \in [S^1_{h,0,ID}(\mathcal{T}_h)]^3 \) and all \( q^h \in S^1(\mathcal{T}_h) \)
\[
A_{NS}(v^h, q^h; u^h, p^h) + S_{BBVMS}(v^h, q^h; u^h, p^h) = F_{NS}(v_h)
\]
with the bilinear form of the NSB equations
\[
A_{NS}(v^h, q^h; u^h, p^h) =
\int_{\Omega} \rho \, v^h \cdot \left[ \left( \frac{\partial u^h}{\partial t} + (u^h - w) \cdot \nabla u^h + \frac{v}{K} (u^h - u^h_s) \right) + \varepsilon(v^h) : \sigma(u^h, p^h) \right] \, dx
\]
\[- \int_{\Gamma_{\text{outflow}}} \rho \beta((u^h - w) \cdot n)_- \cdot v^h \cdot u^h \, ds_x + \int_{\Omega} q^h \nabla \cdot u^h \, dx,
\]
the bilinear form $S_{RBVMS}$, which will be explained later in Equation (21), and the right hand side contribution

$$F_{NS} = -p_{WK} \int_{\Gamma_{\text{outflow}}} \mathbf{n} \cdot \mathbf{v}_h \, ds.$$

We use standard notation to describe the finite element function space $[S_{\text{h,g,}\Gamma_D}(\mathcal{T}_N)]^3$ as a conformal vector-valued trial space of piece-wise linear, globally continuous basis functions $\mathbf{v}_h$ over a tessellation $\mathcal{T}_N$ of $\Omega$ into $N$ finite elements constrained by $\mathbf{v}_h = \mathbf{g}$ on Dirichlet boundaries, more precisely

$$[S_{\text{h,g,}\Gamma_D}(\mathcal{T}_N)]^3 := \{ \mathbf{v}_h \in [C(\mathcal{T}_N)]^3 : \mathbf{v}_h|_{\Omega} \in [P^1(\tau)]^3 \forall \tau \in \mathcal{T}_N \land \mathbf{v}_h|_{\Gamma_D} = \mathbf{g} \},$$

$$S_{\text{h}}(\mathcal{T}_N) := \{ q_h \in C(\mathcal{T}_N) : q_h|_{\Omega} \in P^1(\tau) \forall \tau \in \mathcal{T}_N \},$$

where for this work $\Gamma_D := \Gamma_{\text{noslip}} \cup \Gamma_{\text{inflow}}$. For further details we refer to [S10, S40]. As previously described in [S26] we utilize the residual based variational multiscale (RBVMS) formulation as proposed in [S7, S8], providing turbulence modeling in addition to numerical stabilization. In the following we give a short summary of the changes necessary to use RBVMS methods for the ALE-NSB equations. Briefly, the RBVMS formulation is based on a decomposition of the solution and weighting function spaces into coarse and fine scale subspaces and the corresponding decomposition of the velocity and their respective test functions. Henceforth the fine scale quantities and their respective test functions shall be denoted with the superscript ‘’. We assume $\mathbf{u}_c = \mathbf{u}_c^h$, quasi-static fine scales ($\frac{\partial \mathbf{u}_c}{\partial t} = 0$), as well as $\frac{\partial \mathbf{u}_c}{\partial t} = 0$, $\mathbf{u}' = 0$ on $\partial \Omega(t)$ and incompressibility conditions for $\mathbf{u}_c$ and $\mathbf{u}'$. The fine scale pressure and velocity are approximated in an element-wise manner by means of the residuals $r_M$ and $r_C$.

$$\mathbf{u}' = -\frac{r_{\text{SUPS}}}{\rho} r_M(\mathbf{u}_c^h, \rho^h)$$  \hspace{1cm} (17)

$$\rho' = -\rho \cdot v_{\text{LSIC}} r_C(\mathbf{u}_c^h)$$  \hspace{1cm} (18)

The residuals of the NSB equations and the incompressibility constraint are:

$$r_M(\mathbf{u}_c^h, \rho^h) = \rho \frac{\partial}{\partial t} \mathbf{u}_c^h + \rho(\mathbf{u}_c^h - \mathbf{w}) \cdot \nabla \mathbf{u}_c^h - \nabla \cdot \mathbf{\sigma}(\mathbf{u}_c^h, \rho^h) + \frac{\mu}{K}(\mathbf{u}_c^h - \mathbf{u}_c^h)$$  \hspace{1cm} (19)

$$r_C(\mathbf{u}_c^h) = \nabla \cdot \mathbf{u}_c^h$$  \hspace{1cm} (20)

Taking all assumptions into consideration and employing the scale decomposition followed by partial integration yields the bilinear form of the RBVMS formulation $S_{RBVMS}(\mathbf{v}_c^h, q_c^h; \mathbf{u}_c^h, \rho_c^h)$,

$$S_{RBVMS}(\mathbf{v}_c^h, q_c^h; \mathbf{u}_c^h, \rho_c^h) =$$

$$+ \sum_{\Omega_e \in \mathcal{T}_N} \int_{\Omega_e} r_{\text{SUPS}} \left( (\mathbf{u}_c^h - \mathbf{w}) \cdot \nabla \mathbf{v}_c^h + \frac{1}{\rho} \nabla q_c^h - \frac{1}{\rho} \nabla \mathbf{v}_c^h \right) r_M(\mathbf{u}_c^h, \rho^h) \, dx$$

$$+ \sum_{\Omega_e \in \mathcal{T}_N} \int_{\Omega_e} \rho \cdot v_{\text{LSIC}} \nabla \cdot \mathbf{v}_c^h r_C(\mathbf{u}_c^h) \, dx$$

$$- \sum_{\Omega_e \in \mathcal{T}_N} \int_{\Omega_e} r_{\text{SUPS}} \mathbf{v}_c^h \cdot \left( r_M(\mathbf{u}_c^h, \rho^h) \cdot \nabla \mathbf{u}_c^h \right) \, dx$$

$$- \sum_{\Omega_e \in \mathcal{T}_N} \int_{\Omega_e} \frac{r_{\text{SUPS}}}{\rho} \nabla \mathbf{v}_c^h : (r_M(\mathbf{u}_c^h, \rho^h) \otimes r_M(\mathbf{u}_c^h, \rho^h)) \, dx.$$

The residuals (19) and (20) are evaluated for every element $\Omega_e \in \mathcal{T}_N$. Following [S37] the stabilization parameters $r_{\text{SUPS}}$ and $v_{\text{LSIC}}$ are defined as:
\[ \tau_{\text{SUPS}} := \left( \frac{4}{\Delta t^2} + (u^h - w) \cdot G(u^h - w) + \left( \frac{v}{K} \right)^2 + C_j v^2 G \cdot G \right)^{-\frac{1}{2}} \]

(22)

\[ \nu_{\text{LSIC}} := \frac{1}{iv(G) \tau_{\text{SUPS}}} \]

(23)

Here \( G \) is the three dimensional element metric tensor defined per finite element as \( G|_{\Gamma} := J^{-1}_i J_{i}^{-T} \), with \( J_i \) being the Jacobian of the transformation of the reference element to the physical finite element \( \tau_i \in T_N \). \( \Delta t \) denotes time step size and \( C_j \) is a positive constant, taken as 30, derived from an element-wise inverse estimate. For further details see \([S7,S8]\).

S.I.C. Numerical Solution Strategy

Spatio-temporal discretization of all PDEs and the solution of the arising systems of equations relied upon the Cardiac Arrhythmia Research Package (CARPentry), see \([S73]\). For temporal discretization of the ALE-NSB equations we used the generalized-\( \alpha \) method, see \([S23]\) with a spectral radius \( \rho_{\infty} = 0.2 \). For updating the Windkessel pressures \( p_{WK} \) we discretized \([11]\) with an implicit Euler method. For ease of coupling with our CFD solver the calculation of \( \Omega(t) \) in \([13]\) is lagged by one Newton iteration. After discretization in space as described in Section S.I.B and temporal discretization using the generalized-\( \alpha \) integrator we obtain a nonlinear algebraic system to solve for advancing time from timestep \( t_n \) to \( t_{n+1} \). A quasi inexact Newton-Raphson method is used to solve this system with linearization approach similar to \([S8]\) adapted to the NSB equations. At each iteration a block system of the form

\[
\begin{bmatrix}
K_h & B_h & \Delta u \\
C_h & D_h & \Delta p
\end{bmatrix}
\begin{bmatrix}
\Delta u \\
\Delta p
\end{bmatrix}
= -\begin{bmatrix}
-R_{\text{upper}} \\
-R_{\text{lower}}
\end{bmatrix},
\]

is solved with \( K_h, B_h, C_h, \) and \( D_h \) denoting the Jacobian matrices, \( \Delta u, \Delta p \) representing the velocity and pressure updates and \( R_{\text{upper}}, R_{\text{lower}} \) indicating the residual contributions. In this regard we use the flexible generalized minimal residual method (fGMRES) and efficient preconditioning based on the PCFIELDSPLIT\(^1\) package from the library PETSc \([S4,S6]\) and the incorporated suite HYPRE BoomerAMG \([S19]\). By extending our previous work \([S3,S26,S27]\) we implemented the methods in the finite element code Cardiac Arrhythmia Research Package (CARPentry) \([S42,S43]\).

S.II. Obstacle Representation

Here we want to give a brief description of how we represent moving obstacles for usage in the ALE-NSB equations. This task is solved by representing obstacles using triangular surface meshes followed by element-wise calculation of the partial volume covered by the obstacle. In the first step, all nodes within the obstacle are identified using the ray casting algorithm \([S18,S33]\). Subsequently, all elements are split into three categories and receive a corresponding volume fraction value \( \nu_f \), describing the partial volume covered by the obstacle:

- Elements fully covered by the obstacle lie in \( \Omega_s \), consequently \( \nu_f = 1 \).
- Elements outside the obstacle lie in \( \Omega_f \) and obtain \( \nu_f = 0 \).
- Elements that are split by the element surface correspond to elements in \( \Omega_p \), hence

\[ \nu_f = \frac{V_{in}}{V_{tot}} \]

(24)

\(^1\)https://www.mcs.anl.gov/petsc/petsc-current/docs/manualpages/PC/PCFIELDSPLIT.html
where $V_{in}$ denotes the element volume covered by the obstacle and $V_{tot}$ is the total element volume.

This procedure is carried out for every time step and yields a time-dependent, element-based volume fraction distribution $v_f(t, x)$, that serves as a basis to provide a suitable permeability distribution, see Figure S1. In this work we define $\frac{1}{K(t, x)} := \frac{v_f(t, x)}{\kappa}$ with $\kappa$ being a fixed penalization factor, e.g. $\kappa = 10^{-8}$. All permeability distributions in this work have been generated using the open-source software Meshtool\[^{2}\] see [S36] and [S17] for algorithmic details. In the case of obstacles that change from open to closed state over time we use a simple scaling function. For example, assume an obstacle representing a heart valve region will be open at a time instance $t_{op}$ and it takes $\text{dur}_V$ time to switch from open to closed we define

$$
\chi(t) := \begin{cases} 
\frac{t_{op} - t}{\text{dur}_V} & t \in [t_{op} - \text{dur}_V, t_{op}] \\
0 & t \in [t_{op}, t_{cl} - \text{dur}_V] \\
\frac{t - t_{cl} - \text{dur}_V}{\text{dur}_V} & t \in [t_{cl} - \text{dur}_V, t_{cl}] \\
1 & \text{else}
\end{cases},
$$

and modify $\frac{1}{K(t, x)}$ to $\frac{\chi}{K(t, x)}$.

![Figure S1: Schematic representation of the $v_f$ distribution associated to an obstacle, which is represented by the red line, at a fixed point time $t$.](https://bitbucket.org/aneic/meshtool/src/master/)

**S.III. Computation of Residence Times on Moving Domains**

Here we will give a brief outline of the methods and algorithms used to compute residence time distributions. The starting point is the following PDE describing the time evolution of a residence time distribution field originating from [S14 S31]. Given a moving fluid domain $\Omega(t) \subset \mathbb{R}^3$ [s] and a region of interest $V(t) \subset \Omega(t)$ the evolution of the time $\tau(t, x)$ spent in $V$ by an arbitrarily small fluid particle

[^2]: https://bitbucket.org/aneic/meshtool/src/master/
caught at point \( x \in \Omega(t) \) at time \( t \) can be described as

\[
\frac{\partial}{\partial t} \tau + (u - w) \cdot \nabla \tau - \epsilon \Delta \tau = H(t, \mathbf{x}) \quad \text{in } \Omega(t),
\]

\[
\frac{\partial}{\partial n} \tau = 0 \quad \text{on } \Gamma_N(t),
\]

\[
\tau = g \quad \text{on } \Gamma_D(t),
\]

\[
H(t, \mathbf{x}) := \begin{cases} 
1 & \text{if } (t, \mathbf{x}) \in V(t), \\
0 & \text{else}
\end{cases}
\]

with the fluid velocity \( u \), the ALE mesh velocity \( w \) and a small artificial diffusion parameter \( \epsilon \) \([\text{m}^2\text{s}^{-1}]\) added for numerical stability of the method. For this work we have used \( \epsilon = 1 \times 10^{-12} \). The fluid velocity \( u \) as well as the ALE mesh velocity \( w \) are assumed to be given functions, e.g. coming from a pre-computed CFD simulation. In our applications we set \( \Gamma_D(t) = \emptyset \) and \( \Gamma_N(t) = \partial \Omega(t) \). Furthermore, the region of interest \( V(t) \) is assumed as a time-evolving tag region assigned to a particular anatomic region, e.g.: ventricular blood pools, and left atrial appendage respectively. After discretization we have

\[
M_h(t) \dot{\tau} + K_h(t) \tau(t) = F_h(t) \tag{26}
\]

with

\[
M_{h,ij}(t) = \int_{\Omega(t)} \phi_i(t) \phi_j(t) \, dx,
\]

\[
K_{h,ij}(t) = \epsilon \int_{\Omega(t)} \nabla \phi_i(t) \cdot \nabla \phi_j(t) \, dx
\]

\[
\quad + \int_{\Omega(t)} (u(t) - w(t)) \cdot \nabla \phi_i(t) \phi_j(t) \, dx,
\]

\[
F_{h,j}(t) = \int_{V(t)} \phi_j(t) \, dx,
\]

with \( \{\phi_i(t)\}_{i=0}^n \) being the time-dependent test and trials functions in the ALE domain. For regular domain movement it is safe to assume that \( M_h(t) \) is invertible for all \( t \) and we can rewrite (26) as

\[
\dot{\tau} + M_h^{-1}(t) K_h(t) \tau(t) = M_h^{-1}(t) F_h(t). \tag{27}
\]

Next, we apply the modified Crank-Nicholson scheme in time as proposed in [S15] giving

\[
\left( M_c + \frac{\Delta t}{2} K \right) \tau^{n+1} = \left( M_c - \frac{\Delta t}{2} K \right) \tau^n + \frac{\Delta t}{2} F,
\]

where we used the following shorthand notation

\[
M_c := M_h(t^{n+\frac{1}{2}}),
\]

\[
K := K_h(t^{n+\frac{1}{2}}),
\]

\[
F := F_h(t^{n+\frac{1}{2}}).
\]
Equation (28) is our starting point for applying the FCT scheme similar to [S25]. Following the ideas of FEM-FCT methods we define the matrices

\[
L := K + D,
\]

\[
D_{ij} := \begin{cases} 
-\max \{0, K_{ij}, K_{ji}\} & \text{if } i \neq j, \\
-\sum_{j=1, j \neq i}^{N} D_{ij} & \text{else},
\end{cases}
\]

\[
M_L := \text{diag}(m),
\]

\[
m_i := \sum_{j=1}^{N} M_{C,ij}.
\]

The construction of \( L \) ensures zero row and column sums. Instead of (28) we consider

\[
\left( M_L + \frac{\Delta t}{2} L \right) \tau^{n+1} = \left( M_L - \frac{\Delta t}{2} L \right) \tau^n + \frac{\Delta t}{2} F, \tag{29}
\]

which represents a stable low-order scheme whose solution doesn’t possess any over or undershoots but suffers from to smeared layers. To correct this behavior and artificial flux correction vector \( f^*(\tau^{n+1}, \tau^n) \) is added to the right hand side of (29). The definition of \( f^* \) follows from an ad-hoc ansatz

\[
f_i^*(\tau^{n+1}, \tau^n) = \sum_{j=1}^{n} \alpha_{ij} r_{ij},
\]

with the fluxes \( r_{ij} \) defined as

\[
r_{ij} := M_{C,ij}(\tau_i^{n+1} - \tau_j^{n+1}) - M_{C,ij}(\tau_i^n - \tau_j^n)
\]

\[-\frac{\Delta t}{2} D_{ij}(\tau_i^{n+1} - \tau_j^{n+1}) - \frac{\Delta t}{2} D_{ij}(\tau_i^n - \tau_j^n), \tag{30}
\]

and weights \( \alpha_{ij} \in [0, 1] \). The representation for \( r_{ij} \) follows from first subtracting (28) from (29) and applying the properties of the matrices \( M_C \) and \( D \). This formulation represents a nonlinear system. In [S25] a linear variant has been proposed which we adapted to the moving-domain case. For this we use the explicit solution \( \tilde{\tau} \) to (29), by means of an explicit Euler scheme approximating the solution \( \tau^{n+\frac{1}{2}} \) at time step \( t_n + \frac{\Delta t}{2} \), reading

\[
\tilde{\tau} := \tau^n - \frac{\Delta t}{2} M_L^{-1} (L \tau^n - F).
\]

Inserting \( \tilde{\tau} \) into (30) and rearranging terms yields

\[
r_{ij} = \frac{\Delta t}{2} \left( M_{C,ij}(\eta_i^{n+\frac{1}{2}} - \eta_j^{n+\frac{1}{2}}) - D_{ij}(\tilde{\tau}_i - \tilde{\tau}_j) \right),
\]

where \( \eta_i^{n+\frac{1}{2}} := (M_L^{-1}(F - L \tau^n))_i \). Additionally, as suggested in [S29], we employ prelimiting in the form

\[
r_{ij} = 0 \quad \text{if } r_{ij}(\tilde{\tau}_i - \tilde{\tau}_j) < 0.
\]

The computation of the weights \( \alpha_{ij} \) follows the same procedure as in [S25] using Zalesak’s algorithm [S44]. We also refer to [S29][S30] for a more detailed overview of the presented method. Computation of the residence time distribution fields have been included as addon in CARPentry. After computation of the residence time distribution \( \tau \) we can calculate the residence time RT spend in \( V(t) \) over a time period \((t_0, t_1)\) as

\[
\text{RT} := \frac{1}{(t_1 - t_0)|V|} \int_{t_0}^{t_1} \int_{\Omega(t)} \tau(t, x) H(t, x) \, dx dt,
\]

\[
|V| := \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \int_{\Omega(t)} H(t, x) \, dx dt.
\]
Figure S2: Time-averaged residence time distributions $\tau_{AVG}$ with $V(t)$ defined through different labels in the computational mesh. Time average taken over the final two heartbeats with beatlength equal to 0.725 s.

Figure S2 and Figure S3 show illustrations of time averaged residence time distributions that were generated for this work as part of the sensitivity analysis.

S.IV. Pope’s Criterion of Turbulence Resolution

In LES type formulations the resolved velocity field is fundamentally linked to the numerical method used, hence there is no notion of convergence to the solution of a partial differential equation. This leads to the problem that mesh convergence often cannot be established by the classical methods. To remedy this problem proposes the use of a measure of turbulence resolution $M$, utilizing the fraction of turbulent kinetic energy resolved by the grid in question. In order to obtain a point-wise measure, rather than the kinetic energy itself, the kinetic energy density $K(x, t)$ is considered:

$$K(x, t) = \rho \frac{1}{2} \left( u(x, t)^2 \right).$$

The resulting point-wise measure of turbulence resolution $M$ reads:

$$M(x, t) = \frac{K'(x, t)}{K_{tot}(x, t)}.$$  \hfill (32)

Here $K'$ is the turbulent kinetic energy of the residual motions, hence of the motions not resolved by the grid, and $K_{tot}$ stands for the total kinetic energy. $K_{tot}$ may be written as the sum of the resolved turbulent kinetic energy $K^h$ and the not resolved turbulent kinetic energy $K'$:

$$K_{tot}(x, t) = K^h(x, t) + K'(x, t).$$  \hfill (33)

The resolved turbulent kinetic energy $K^h$ is calculated from (31) using the fluctuating part of the resolved fluid velocity $u_f$, which is given by:

$$u_f(x, t) = \overline{u^h(x, t)} - \bar{u}^h(x, t),$$  \hfill (34)
Figure S3: Time-averaged residence time distributions $\tau_{RV}^{AVG}$ with $V(t)$ defined as right ventricular blood pool in the computational mesh. Time average taken over the final two heartbeats with beatlength equal to 0.725 s.

where $\bar{u}^h$ is an average with respect to time. When considering a constant inflow $\bar{u}^h$ is given by the standard mean over all time steps ($t = 1 \ldots T$, hence $\bar{u}^h$ is not time-dependent):

$$\bar{u}^h(x) = \frac{1}{T} \sum_{t=1}^{T} u^h(x, t)$$

(35)

In the case of a pulsatile behavior however a phase average is considered:

$$\bar{u}^h(x, t) = \frac{1}{n} \sum_{k=0}^{n-1} u^h(x, t + k\tau),$$

(36)

where $n$ is the number of cycles or beats and $\tau$ is the period or beat length. By the use of (32) a criterion for sufficient mesh resolution is given:

$$M(x, t) \leq \epsilon_M$$

(37)

In [538] a value of $\epsilon_M = 0.2$ is proposed, which corresponds to requiring a minimum of 80% of the total turbulence energy to be resolved.

We calculated this criterion based on the simulation of four beats for different spatial and temporal resolutions with average edge lengths of $\Delta x = 3000, 1500, 750 \mu m$ and time step sizes of $\Delta t = 1450, 725, 362.5$ ms for the mesh of the left heart. Figure S4 shows a comparison of the average Pope criterion, with average taken over all elements of the mesh. From this we concluded that the mesh with average edge length of $\Delta x = 750 \mu m$ and a time step size $\Delta t = 362.5$ ms was sufficient to resolve the flow dynamics in the left heart. For reasons of practicality we used the same average edge length and time step size for the right side heart.

**S.V. Input Parameter Variance Effect on Output Features**

This serves as additional interpretation for the results in the main manuscript. Figure S5 shows the extracted temporal signals of all parameter sets for the pressure differences $\Delta p_{MV1,2,3,4}$ in the LA. While
Figure S4: Average Pope criterion for the different spatial and temporal discretization levels. The average is taken over all elements in the mesh.

there is no strong influence on the output in systole, one can see a clear variation in the outputs in diastole.

S.VI. 5-Fold Cross-Validation Results

Table S1 and Table S2 summarize the results of the cross-validation. Features with an average $R_2$-score of $< 0.5$ were excluded from global sensitivity analysis in this work. It can be observed that the $R_2$ scores are on average lower for left heart features. We attribute that to the increased turbulence in left heart blood flow compared to right heart blood flow.

S.VII. Comparing Influence of Time Step Size on Main Vortex Center in the Left Ventricle

To study the influence of time step size on the accuracy of vortex formation we ran a simulation of left heart blood flow with successive refined time step sizes $\Delta t = 362.5, 181.25, 90.625$ ms. It is known, see [S28] and references therein, that vorticity is not a suitable criterion for vortex identification, hence we used the scaled Q-criterion $Q_s$ defined as

$$Q_s := \frac{1}{2} \left( \frac{\| \Omega \|_{F}^2}{\| S \|_{F}^2} - 1 \right),$$

$$\Omega := \frac{1}{2} \left( \nabla u - \nabla u^\top \right),$$

$$S := \frac{1}{2} \left( \nabla u + \nabla u^\top \right),$$

$$\| A \|_{F}^2 := \sum_{i,j=1}^{3} A_{ij}^2.$$
Figure S5: Extracted time signals for pressure differences in the LA for the second heart beat. Diastole is indicated by the shaded blue area in the plots.

Table S1: $R_2$-Scores for cross validation of LV features.

| Feature   | $R_2$-Scores | Average |
|-----------|--------------|---------|
|           | Fold 1    | Fold 2    | Fold 3    | Fold 4    | Fold 5    |
| $\Delta p_{AV}$ | 0.96    | 0.97    | 0.95    | 0.96    | 0.87    | 0.94    |
| $\Delta p_{MV}$ | 0.89    | 0.97    | 0.96    | 0.96    | 0.89    | 0.93    |
| $\Delta p_{MV1}$ | 0.57    | 0.47    | 0.61    | 0.49    | 0.53    | 0.53    |
| $\Delta p_{MV2}$ | 0.31    | 0.41    | 0.48    | 0.42    | 0.49    | 0.42    |
| $\Delta p_{MV3}$ | 0.34    | 0.05    | 0.52    | 0.30    | 0.05    | 0.25    |
| $\Delta p_{MV4}$ | 0.45    | 0.51    | 0.48    | 0.48    | 0.61    | 0.51    |
| $\Delta p_{AMV}$ | 0.49    | 0.66    | 0.45    | 0.55    | 0.56    | 0.54    |
| $\Delta p_{AV}$ | 0.19    | 0.44    | 0.65    | 0.91    | 0.56    | 0.55    |
| $\Delta p_{AVMV}$ | 0.63    | 0.72    | 0.65    | 0.82    | 0.63    | 0.69    |
| $E_{k,LV}$ | 0.71    | 0.72    | 0.81    | 0.86    | 0.90    | 0.80    |
| $E_{k,AO}$ | 0.68    | 0.68    | 0.73    | 0.72    | 0.67    | 0.70    |
| $E_{k,LA}$ | 0.92    | 0.90    | 0.79    | 0.88    | 0.89    | 0.88    |
| $RT_{LV}$ | 0.39    | 0.73    | 0.27    | 0.61    | 0.53    | 0.51    |
| $RT_{LAAPP}$ | 0.83    | 0.89    | 0.79    | 0.89    | 0.87    | 0.85    |
| $maxv_{AV}$ | 0.85    | 0.89    | 0.74    | 0.80    | 0.85    | 0.83    |
| $maxv_{MV}$ | 0.46    | 0.71    | 0.06    | -0.18   | -0.15   | 0.18    |
Table S2: $R_2$-Scores for cross validation of RV features.

| Feature        | $R_2$-Scores Average | Fold 1 | Fold 2 | Fold 3 | Fold 4 | Fold 5 |
|----------------|----------------------|--------|--------|--------|--------|--------|
| $\Delta PV$    | 0.99                 | 0.99   | 0.99   | 0.98   | 0.96   | 0.98   |
| $\Delta TV$    | 0.96                 | 0.95   | 0.91   | 0.94   | 0.95   | 0.94   |
| $\Delta TV_1$  | 0.97                 | 0.97   | 0.97   | 0.98   | 0.98   | 0.97   |
| $\Delta TV_2$  | 0.98                 | 0.94   | 0.97   | 0.99   | 0.98   | 0.97   |
| $\Delta TV_3$  | 0.96                 | 0.94   | 0.95   | 0.97   | 0.97   | 0.96   |
| $\Delta ATV$   | 0.78                 | 0.90   | 0.93   | 0.81   | 0.96   | 0.88   |
| $\Delta APA$   | 0.43                 | 0.50   | 0.92   | 0.59   | 0.65   | 0.62   |
| $\Delta PATV$  | 0.99                 | 0.99   | 0.99   | 0.99   | 0.99   | 0.99   |
| $E_{RV}k$      | 0.96                 | 0.96   | 0.99   | 0.99   | 0.99   | 0.97   |
| $E_{PA}k$      | 0.98                 | 0.98   | 0.96   | 0.98   | 0.98   | 0.98   |
| $E_{RA}k$      | 0.92                 | 0.96   | 0.93   | 0.98   | 0.92   | 0.94   |
| $RT_{RV}$      | 0.98                 | 0.99   | 0.91   | 0.95   | 0.94   | 0.95   |
| maxv$_{PV}$    | 0.98                 | 0.89   | 0.93   | 0.94   | 0.87   | 0.92   |
| maxv$_{TV}$    | 0.98                 | 0.92   | 0.91   | 0.94   | 0.79   | 0.91   |

For this value. Afterwards, we extracted the major vortex component in the left ventricle at peak diastole and calculated the vortex centers for each time discretization. Table S3 shows a comparison of the relative error of the identified vortex centers and Figure S6 shows a visual comparison of the resulting isosurfaces. From this results we concluded that our simulations accurately resolved the vortices at the chosen time step size of $\Delta t = 362.5$ ms coinciding with the results obtained from using Pope’s criterion as described in section S.IV.

Table S3: Results for Vortex Center Identification.

| $\Delta t$ [ms] | Vortex Center | rel. Error [%] |
|-----------------|---------------|----------------|
|                 | x [mm] | y [mm] | z [mm] |
| 362.5           | -67.40 | 191.162 | 1889.86 | 0.17 |
| 181.25          | -67.81 | 190.369 | 1889.88 | 0.15 |
| 90.625          | -70.39 | 191.572 | 1890.95 | —    |

S.VIII. Scatterplot of the Locations of Failing Samples

Here we include a projection of the training data set used for calibrating the left heart GPEs overlayed with the samples that led to failed simulations. From the result in Figure S7 we conclude that the failed samples appear to be random samples.

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Figure S6: Comparison of the major vortex centers extracted from isosurfaces of the scaled Q-criterion $Q_s$ at value 2.5 at peak diastole for different time discretizations: a) $\Delta t = 362.5\text{ms}$ (orange) and reference time step $\Delta t = 90.625\text{ms}$ (green), and b) $\Delta t = 181.25\text{ms}$ (orange) and reference time step $\Delta t = 90.625\text{ms}$ (green). Additionally the vortex centers are depicted as colored spheres in orange and green.
Figure S7: 2D Projection of the Latin Hypercube Sampling used for training the GPEs. Blue markers depict all training points, while orange markers show the samples leading to failed simulations.

Sample dimension = 90 points
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