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Data-driven kinematics-consistent model order reduction of fluid-structure interaction problems: application to deformable microcapsules in a Stokes flow

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In this paper, we present a generic approach of a dynamical data-driven model order reduction technique for three-dimensional fluid-structure interaction problems. A low-order continuous linear differential system is identified from snapshot solutions of a high-fidelity solver. The reduced order model (ROM) uses different ingredients like proper orthogonal decomposition (POD), dynamic mode decomposition (DMD) and Tikhonov-based robust identification techniques. An interpolation method is used to predict the capsule dynamics for any value of the governing non-dimensional parameters that are not in the training database. Then a dynamical system is built from the predicted solution. Numerical evidence shows the ability of the reduced model to predict the time-evolution of the capsule deformation from its initial state, whatever the parameter values. Accuracy and stability properties of the resulting low-order dynamical system are analysed numerically. The numerical experiments show a very good agreement, measured in terms of modified Hausdorff distance between capsule solutions of the full-order and low-order models both in the case of confined and unconfined flows. This work is a first milestone to move towards real time simulation of fluid-structure problems, which can be extended to non-linear low-order systems to account for strong material and flow non-linearities. It is a valuable innovation tool for rapid design and for the development of innovative devices.

Key words: Fluid-structure interaction, deformable capsule, dynamical system, reduced order model, non-intrusive, data-driven, dynamic mode decomposition

1. Introduction

Fluid-structure interaction (FSI) problems often occur in Engineering (aircraft and automotive industries, wind turbines) as well as in medical applications (cardiovascular systems,

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33 artificial organs, artificial valves, medical devices, etc.). Today the design of such systems
34 usually requires advanced studies and high-fidelity (HF) numerical simulations become
35 an essential tool of computed-aided analysis. However, computational FSI is known to
36 be very time-consuming even when using high-performance computing facilities. Usually,
37 engineering problems are parameterized and the search of suitable designs require numerous
38 computer experiments leading to prohibitive computational times. For particular applications
39 such as the tracking of drug carrier capsules flowing in blood vessels, it would be ideal to
40 have real-time simulations for a better understanding of the behaviour of the dynamics and
41 for efficiency assessment. Unfortunately, today high-fidelity real-time FSI simulations are far
42 from being reached with current High Performance Computing (HPC) facilities.

43 A current trend is to use machine learning (ML) or artificial intelligence (AI) tools such
44 as artificial neural networks (ANN). Such tools learn numerical simulations from HF solvers
45 and try to map entry parameters with output criteria in an efficient way, with response times
46 far less than HF ones, say 3 or 4 orders of magnitude smaller. In some sense, heavy HF
47 computations and training stage are done in an offline stage, and learned ANNs can be used
48 online for real time evaluations and analysis. However, ML and ANN today are not fully
49 satisfactory for dynamical problems, and/or the training stage itself may be time consuming,
50 thus requiring more Central Processing Unit (CPU) time. Another option is the use of
51 model order reduction (MOR). Reduced-order modelling (ROM) can be seen as a 'grey-box'
52 supervised ML methodology, taking advantage of the expected low-order dimensionality of
53 the FSI mechanical problem. By 'grey-box' we mean that the low-dimensional encoding of the
54 ML process is based on mechanical principles and a man-made preliminary dimensionality
55 reduction study. This allows one for a better control of the ROM accuracy and behaviour.
56 There are two families of MOR: intrusive and non-intrusive approaches. The intrusive
57 approaches use physical equations. The low-order model is derived by setting the physical
58 problem on a suitable low-dimensional space. The accuracy can be very good, but the price
59 to pay is the generation of a new code which can be a tedious and long task. The non-intrusive
60 approach does not require heavy code development. It is based on HF simulation results used
61 as entry data. Although it is not based on high-fidelity physical equations, a non-intrusive
62 approach can include a priori physical informations, like e.g. meaningful physical features,
63 prototype of system of equations, pre-computed principal components, consistency with
64 physical principles, etc.

65 In the recent literature, efficient intrusive ROMs for FSI have been proposed e.g. in
66 (Quarteroni *et al.* 2016). But to our knowledge there are far less contributions in non-intrusive
67 ROMs dedicated to FSI.

68 In this paper, we propose a data-driven model order reduction approach for FSI problem
69 which is consistent with the equations of kinematics and is designed from a low-order
70 meaningful system of equations. As case of study, we focus on the motion of a microcapsule,
71 a droplet surrounded by a membrane, subjected to a confined and unconfined Stokes flow.

72 Artificial microcapsules can be used in various industrial applications such as in cos-
73 metics (Miyazawa *et al.* 2000; Casanova & Santos 2016), food industry (Yun *et al.* 2021)
74 and biotechnology, where drug targeting is a high potential application (Ma & Su 2013;
75 Abuhamdan *et al.* 2021; Ghiman *et al.* 2022). Once in suspension in an external fluid,
76 capsules are subjected to hydrodynamics forces, which may lead to large membrane
77 deformation, wrinkle formation or damage. The numerical model must be able to capture
78 the time-evolution of the non-linear 3D large deformations of the capsule membrane.
79 Different numerical strategies are possible to solve the resulting large systems of equations
80 (Lefebvre & Barthès-Biesel 2007; Hu *et al.* 2012; Ye *et al.* 2017; Tran *et al.* 2020). However,
81 they all have long computational times.

82 Different approaches have been used over the past decade to accelerate the computations,

83 such as HPC (e.g. Zhao *et al.* (2010)) and Graphics Processing units (e.g. Matsunaga *et al.*
 84 (2014)). More recently, reduced order models have been proposed to predict the motion
 85 of capsules suspended in an external fluid flow. In Quesada *et al.* (2021), the authors used
 86 the large amount of data generated by numerical simulations to show how relevant it is to
 87 recycle these data to produce lower-dimensional problem using physics-based reduced order
 88 models. However, their method can only predict the steady-state capsule deformed shape.
 89 Boubehziz *et al.* (2021) show for the first time the efficiency of data-driven model-order
 90 reduction technique to predict the dynamics of the capsule in a microchannel. However, the
 91 method is cumbersome as it requires two bases, one to predict the velocity field, the other to
 92 capture the shape evolution over time. And then they reconstruct the solution in the parameter
 93 space thanks to diffuse approximation (DA) strategy.

94 The proposed method serves different objectives. We have designed the method to be
 95 non-intrusive for practical uses of existing high-fidelity FSI solver (also referred to as the
 96 Full-Order Model, or FOM). That means that the ROM methodology should be data-driven.
 97 We also want the ROM to be consistent with the equations of kinematics. The model must
 98 thus return the displacement $\{u\}$ and velocity $\{v\}$ fields from a few snapshots provided by the
 99 FOM. It must otherwise be able to predict the solution for any parameter vector in predefined
 100 admissible domain. Finally, the kinematics-consistent data-driven reduced-order model of
 101 capsule dynamics must ideally open the way to real-time simulations. To do so, we use a
 102 coupling between methods that have been devised to analyse complex fluid problems:

- 103 • Proper Orthogonal Decomposition (POD) (Lumley 1967; Sirovich 1987)
- 104 • Dynamic Mode Decomposition (DMD) (Schmid 2010)

105 along with a Tikhonov regularization for robustness purposes. An interpolation method is
 106 implemented to predict the solution for any values of governing parameters that are not
 107 present in the training database.

108 As indicated above, we mainly consider the case of an initially spherical capsule flowing in a
 109 microfluidic channel with a square cross-section. The corresponding FOM was developed by
 110 Hu *et al.* (2012) and used to get a complete numerical database of the three-dimensional
 111 capsule dynamics as a function of the parameters of the problem: the capsule-to-tube
 112 confinement ratio, hereafter referred to as size ratio a/ℓ and the capillary number Ca , which
 113 measures the ratio between the viscous forces acting onto the capsule membrane and the
 114 membrane elastic forces. For clarity reasons, different ROMs are introduced with increasing
 115 levels of generality, as detailed in Table 1. First, we consider a fixed parameter vector, and get
 116 a space-time ROM in the form of a low-order dynamical system. Next, we generate such N
 117 ROMs for the N parameter samples that fill the admissible parameter domain, and then assess
 118 the uniform accuracy (space-time accuracy over the whole sample set). Finally, we propose a
 119 strategy to derive a general space-time-parameter ROM for any value of the parameter vector
 120 $(Ca, a/\ell)$ in the admissible space. To conclude the results section, we apply the ROM model
 121 to a capsule in a simple shear flow.

122 The paper is organized as follows. First, we present the physics of the problem and the
 123 FOM in Section 2. The strategy used to develop a non-intrusive space-time ROM is detailed
 124 in Section 3. We first present the results for an initially spherical flowing in a square channel.
 125 They first show the results for a given configuration in Section 4, generalize them in Section
 126 5 on the entire database, formed by all the cases that have reached a stationary state and
 127 present in Section 6 the methodology of space-time-parameter ROM. In Section 7, we then
 128 apply the ROM model to a capsule in a simple shear flow before discussing the advantages
 129 and the limits of the method in Section 8.

Nb of parameter samples for data	ROM output type	Verification (accuracy)	Related Section(s) in the paper
1	1 space-time ROM	Space-time accuracy	Sections 3 and 4
N	N space-time ROM	Uniform space-time accuracy on the sample set	Section 5
N	1 space-time-parameter ROM (any parameter couple)	Uniform accuracy	Section 6

Table 1: Stepwise procedure for ROM construction of increasing level of generality.

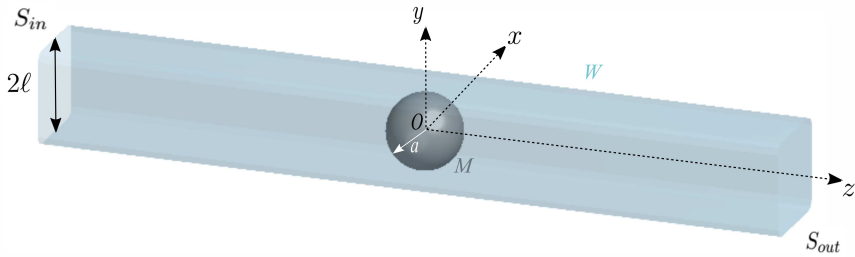


Figure 1: Sketch of the model geometry showing an initially spherical capsule of radius a placed in a channel with a constant square section of side 2ℓ .

2. Full-order microcapsule model, parameters and quantities of interest

2.1. Problem description for a spherical capsule in a channel flow

An initially spherical capsule of radius a flows within a long microfluidic channel having a constant square section of side 2ℓ (Figure 1). The suspending fluid and capsule liquid core are incompressible Newtonian fluids with the same kinematic viscosity η .

The capsule liquid core is enclosed by a hyperelastic isotropic membrane. Its thickness is assumed to be negligible compared to the capsule dimension. The membrane is thus modelled as a surface devoid of bending stiffness with surface shear modulus G_S . The two non-dimensional governing parameters of the problem are the size ratio a/ℓ and the capillary number

$$Ca = \eta V / G_S \quad (2.1)$$

where V is the mean axial velocity of the undisturbed external Poiseuille flow.

The flow Reynolds number is assumed to be very small. We solve the Stokes equations in the external ($\beta = 1$) and internal fluids ($\beta = 2$), together with the membrane equilibrium equation to determine the dynamics of the deformable capsule within the microchannel.

For the fluid problem, we denote $\mathbf{v}^{(\beta)}$, $\boldsymbol{\sigma}^{(\beta)}$ and $p^{(\beta)}$ the velocity, stress and pressure fields in the two fluids. These parameters are non-dimensionalized using ℓ as characteristic

148 length, ℓ/V as characteristic time and $G_S\ell$ as characteristic force. The non-dimensional
149 Stokes equations

$$150 \quad \nabla p^{(\beta)} = Ca\nabla^2 \mathbf{v}^{(\beta)}, \quad \nabla \cdot \mathbf{v}^{(\beta)} = 0, \quad \beta = 1, 2 \quad (2.2)$$

151 are solved in the domain bounded by the cross sections S_{in} at the tube entrance and S_{out}
152 at the exit. These cross sections are assumed to be both located far from the capsule. The
153 reference frame $(O, \mathbf{x}, \mathbf{y}, \mathbf{z})$ is centred at each time step on the capsule center of mass O
154 in the high-fidelity code, but the displacement of the capsule center of mass along the tube
155 axis $O\mathbf{z}$ is computed.

156 The boundary conditions of the problem are the following ones:

- 157 • The velocity field is assumed to be the unperturbed flow field on S_{in} and S_{out} , i.e. the
158 flow disturbance vanish far from the capsule.
- 159 • The pressure is uniform on S_{in} and S_{out} .
- 160 • A no-slip boundary condition is assumed at the channel wall W and on the capsule
161 membrane M :

$$162 \quad \forall \mathbf{x} \in W, \mathbf{v}(\mathbf{x}) = \mathbf{0}; \quad \forall \mathbf{x} \in M, \mathbf{v}(\mathbf{x}) = \frac{\partial \mathbf{u}}{\partial t}. \quad (2.3)$$

- 163 • The normal load \mathbf{n} on the capsule membrane M is continuous, i.e. the non-dimensionalized
164 external load per unit area \mathbf{q} exerted by both fluids is due to the viscous traction jump:

$$165 \quad (\boldsymbol{\sigma}^{(1)} - \boldsymbol{\sigma}^{(2)}) \cdot \mathbf{n} = \mathbf{q} \quad (2.4)$$

166 where \mathbf{n} is the unit normal vector pointing towards the suspending fluid.

167 To close the problem, the external load \mathbf{q} on the membrane is deduced from the local
168 equilibrium equation, which, in absence of inertia, can be written as

$$169 \quad \nabla_s \cdot \boldsymbol{\tau} + \mathbf{q} = \mathbf{0} \quad (2.5)$$

170 where $\boldsymbol{\tau}$ is the non-dimensionalized Cauchy tension tensor (forces per unit arclength in the
171 deformed plane of the membrane) and $\nabla_s \cdot$ is the surface divergence operator. We assume
172 that the membrane deformation is governed by the strain-softening neo-Hookean law. The
173 principal Cauchy tensions can then be expressed as

$$174 \quad \tau_1 = \frac{G_S}{\lambda_1 \lambda_2} \left[\lambda_1^2 - \frac{1}{(\lambda_1 \lambda_2)^2} \right] \quad (\text{likewise for } \tau_2), \quad (2.6)$$

175 where λ_1 and λ_2 are the principal extension ratios measuring the in-plane deformation.

176 *2.2. Numerical procedure*

177 The FSI problem is solved by coupling a finite element method that determines the capsule
178 membrane mechanics with a boundary integral method that solves for the fluid flows
179 (Walter *et al.* 2010; Hu *et al.* 2012). Thanks to the latter, only the boundaries of the flow
180 domain, i.e the channel entrance S_{in} and exit S_{out} , the channel wall and the capsule membrane
181 have to be discretized to solve the problem. The mesh of the initially spherical capsule is
182 generated by subdividing the faces of the icosahedron (regular polyhedron with 20 triangular
183 faces) inscribed in the sphere until reaching the desired number of triangular elements. At
184 the last step, nodes are added at the middle of all the element edges to obtain a capsule mesh
185 with 1280 P_2 triangular elements and 2562 nodes, which correspond to a characteristic mesh
186 size $\Delta h_C = 0.075 a$. The channel mesh of the entrance surface S_{in} and exit surface S_{out}
187 and of the channel wall is generated using `Modulef` (INRIA, France). The central portion
188 of the channel, where the capsule is located, is refined. The channel mesh comprises 3768
189 P_1 triangular elements and 1905 nodes.

190 At time $t = 0$, a spherical capsule is positioned with its center of mass O on the channel

191 axis. At each time step, the in-plane stretch ratio λ_1 and λ_2 are computed from the nodes
 192 deformation. The elastic tension tensor $\boldsymbol{\tau}$ is then deduced from the values of λ_1 and λ_2 .
 193 The finite element method is used to solve the weak form of the membrane equilibrium
 194 equation (2.5) and determine the external load \mathbf{q} .

195 Applying the boundary integral method, the velocity of the nodes on the capsule membrane
 196 reads (Pozrikidis 1992):

$$197 \quad \mathbf{v}(\mathbf{x}) = \mathbf{v}^\infty(\mathbf{x}) - \frac{1}{8\pi\mu_F} \left[\int_M \mathbf{J}(\mathbf{r}) \cdot \mathbf{q} dS(\mathbf{y}) + \int_W \mathbf{J}(\mathbf{r}) \cdot \mathbf{f} dS(\mathbf{y}) - \Delta P \int_{S_{out}} \mathbf{J}(\mathbf{r}) \cdot \mathbf{n} dS(\mathbf{y}) \right] \quad (2.7)$$

198 for any \mathbf{x} in the spatial domain when the suspending and internal fluids have the same
 199 viscosity. The vector \mathbf{f} is the disturbance wall friction due to the capsule, ΔP is the additional
 200 pressure drop and $\mathbf{r} = \mathbf{y} - \mathbf{x}$.

201 To update the position of the membrane nodes, the nodal displacement \mathbf{u} is computed
 202 by integrating equation (2.3) in time. The procedure is repeated until the desired non-
 203 dimensional time VT/ℓ .

204 For later development, it is more convenient to work on the condensed abstract form of
 205 the system. The full order semi-discrete FSI system to solve consists of the kinematics and
 206 the membrane equilibrium algebraic equations:

$$207 \quad \{\dot{\mathbf{u}}\} = \{\mathbf{v}\}, \quad t \in [0, T], \quad (2.8)$$

$$208 \quad \{\mathbf{v}\} = \varphi(\{\mathbf{u}\}) \quad (2.9)$$

where φ is a non-linear mapping from \mathbb{R}^{3d} to \mathbb{R}^{3d} and d is the number of nodes on the
 membrane. Regarding time discretization, a Runge-Kutta Ralston scheme is used:

$$\begin{aligned} \{\widehat{\mathbf{u}}^{n+2/3}\} &= \{\mathbf{u}^n\} + \frac{2}{3}\Delta t \{\mathbf{v}^n\}, \\ \{\widehat{\mathbf{v}}^{n+2/3}\} &= \{\varphi\}(\{\widehat{\mathbf{u}}^{n+2/3}\}), \\ \{\mathbf{u}^{n+1}\} &= \{\mathbf{u}^n\} + \Delta t \left(\frac{1}{4}\{\mathbf{v}^n\} + \frac{3}{4}\{\widehat{\mathbf{v}}^{n+2/3}\} \right), \\ \{\mathbf{v}^{n+1}\} &= \{\varphi\}(\{\mathbf{u}^{n+1}\}), \\ \{\mathbf{u}^0\} &= \{\mathbf{0}\}, \quad \{\mathbf{v}^0\} = \{\varphi\}(\{\mathbf{0}\}) \end{aligned}$$

210 where $\Delta t > 0$ is a constant time step and $\{\mathbf{u}\}^n$ and $\{\mathbf{v}\}^n$ respectively represent the discrete
 211 membrane displacement field and the discrete membrane velocity field at discrete time $t^n =$
 212 $n\Delta t$. The initial condition is simply $\{\mathbf{u}\}^0 = \{\mathbf{0}\}$.

213 The whole numerical scheme is subject to some Courant-Friedrichs-Lewy (CFL) type
 214 stability condition on the time step (Walter et al. 2010) because of its explicit nature. The
 215 numerical method is conditionally stable if the time step Δt satisfies

$$216 \quad \frac{V}{\ell} \Delta t < O \left(\frac{\Delta h_C}{\ell} Ca \right). \quad (2.10)$$

217 From the computational point of view, the resolution of (2.9) at each time step requires i) the
 218 computation of the disturbance wall friction \mathbf{f} at all the wall nodes, ii) the additional pressure
 219 drop ΔP , iii) the traction jump \mathbf{q} at the membrane nodes and iv) the boundary integrals for
 220 each node. The resulting numerical FOM may thus be time-consuming, depending on the
 221 membrane discretization and the number of time steps. Figure 2 shows that the evolution of
 222 the computational cost when $a/\ell = 0.7$, considering the mesh discretization described above
 223 and a workstation equipped with 2 processors Intel[®] Xeon[®] Gold 6130 CPU (2.1 GHz).

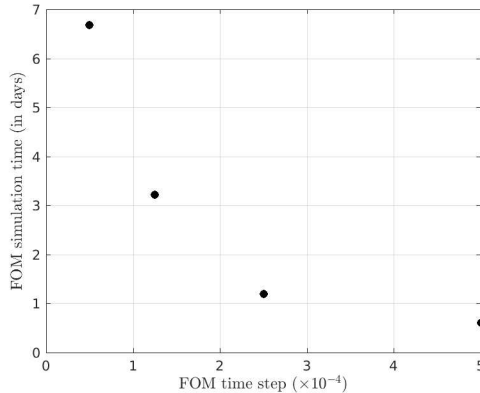


Figure 2: Simulation time of the dynamics of the capsule over a non-dimensional time $Vt/\ell = 10$ ($a/\ell = 0.7$) according to the time step. Simulations were performed on a workstation equipped with 2 processors Intel[®] Xeon[®] Gold 6130 CPU (2.1 GHz).

224 A week of computation is sometimes necessary to simulate the dynamics of an initially
 225 spherical capsule in a microchannel over the non-dimensional time $VT/\ell = 10$.

226 For that reason, a model-order reduction (MOR) strategy is studied in this paper, in order
 227 to reduce the computational time by several orders of magnitude. ROMs try to approximate
 228 solutions of the initial problem by strongly lowering the dimensionality of the numerical
 229 model, generally using a reduced basis (RB) of suitable functions, then derive a low-order
 230 system of equations.

231 In the case of differential algebraic equations (DAE) like (2.8)-(2.9), the reduced system of
 232 equations to find should also be of DAE nature. Remark that it is often possible to reformulate
 233 DAEs as a system of ordinary differential equations (ODEs) (Ascher & Petzold 1998). In the
 234 next section, we give details on the chosen ROM methodology for the particular case and
 235 context of FSI capsule problem.

236 3. Non-intrusive space-time model-order reduction strategy

237 In this section, the parameter couple $\theta = (Ca, a/\ell)$ is fixed, thus we omit the dependency
 238 of the solutions with respect to θ for the sake of simplicity. For the derivation of the ROM
 239 model, we consider the semi-discrete time-continuous version of the FOM, i.e. (2.8)-(2.9).

240 3.1. Dimensionality reduction and reduced variables for displacements and velocities

241 Assume first that, for any $t \in [0, T]$, the discrete velocity field can be accurately approximated
 242 according to the expansion

$$243 \quad \{v\}(t) \approx \sum_{k=1}^K \beta_k(t) \{\phi_k\} \quad (3.1)$$

for some orthonormal modes $\{\phi_k\} \in \mathbb{R}^d$ and real coefficients $\beta_k(t)$. The truncation rank $K \leq d$ is of course expected to be far less than d as expected in a general ROM methodology.

From the kinematics equations we have

$$\begin{aligned}\{u\}(t) &= \int_0^t \{v\}(s) ds \\ &\approx \int_0^t \beta_k(s) \{\phi_k\} ds\end{aligned}$$

244 so that the displacement field can be accurately represented by

$$245 \quad \{u\}(t) \approx \sum_{k=1}^K \alpha_k(t) \{\phi_k\} \quad (3.2)$$

246 where $\alpha_k(t) = \int_0^t \beta_k(s) ds$. The coefficients $(\alpha_k(t))_k$ and $(\beta_k(t))_k$ are called the reduced
247 variables. For the sake of readability and mental correspondence between full-order un-
248 knowns and reduced ones, we will use the convenient notations

$$249 \quad \boldsymbol{\alpha}(t) = (\alpha_1(t), \dots, \alpha_K(t))^T, \quad \boldsymbol{\beta}(t) = (\beta_1(t), \dots, \beta_K(t))^T$$

250 where the exponent T denotes the transpose of the matrix. The condensed matrix forms
251 of (3.2) and (3.1) respectively are

$$252 \quad \{u\}(t) \approx \boldsymbol{Q} \boldsymbol{\alpha}(t), \quad \{v\}(t) \approx \boldsymbol{Q} \boldsymbol{\beta}(t), \quad (3.3)$$

253 where $\boldsymbol{Q} = [\{\phi_1\}, \dots, \{\phi_K\}] \in \mathcal{M}_{dK}$. Since the modes $\{\phi_k\}$ are assumed to be orthonormal
254 (for the standard Euclidean inner product), the matrix \boldsymbol{Q} is a semi-orthogonal matrix, i.e.
255 $\boldsymbol{Q}^T \boldsymbol{Q} = \boldsymbol{I}_K$. In particular, we have $\boldsymbol{\alpha}(t) \approx \boldsymbol{Q}^T \{u\}(t)$ and $\boldsymbol{\beta}(t) = \boldsymbol{Q}^T \{v\}(t)$.

256 Note that the modes $\{\phi_k\}$ and reduced variables $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ are determined for each parameter
257 set $(Ca, a/\ell)$, but a common value of the truncation rank K is chosen for all the sets. Its
258 practical computation will be detailed in a next subsection, as well as that of the modes $\{\phi_k\}$.

259

3.2. ROM prototype

260 The expressions $\{\tilde{u}\}(t) = \boldsymbol{Q} \boldsymbol{\alpha}(t)$ and $\{\tilde{v}\}(t) = \boldsymbol{Q} \boldsymbol{\beta}(t)$ provide low-order representations of
261 displacement and velocity fields respectively. We can now write equations for the reduced
262 vectors $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ respectively. In this subsection, let us consider a projection Galerkin-
263 type approach. Let us denote $\langle \cdot, \cdot \rangle$ the standard Euclidean scalar product in \mathbb{R}^d . Considering
264 a test vector $\{w\}$ in $W = \text{span}(\{\phi_1\}, \dots, \{\phi_K\})$, we look for an approximate displacement
265 field $\{\tilde{u}\}(t)$ solution of the projected kinematics equations

$$266 \quad \left\langle \frac{d}{dt} \{\tilde{u}\}(t), \{w\} \right\rangle = \langle \{\tilde{v}\}(t), \{w\} \rangle \quad \forall \{w\} \in W.$$

267 By considering each test vector $\{w\} = \{\phi_k\}$, we get the consistent reduced kinematics
268 equation

$$269 \quad \dot{\boldsymbol{\alpha}} = \boldsymbol{\beta}. \quad (3.4)$$

270 Consider now the projected field $\{\tilde{v}\}(t)$ which is solution of the system of algebraic equations
271 (Galerkin approach):

$$272 \quad \langle \{\tilde{v}\}(t), \{w\} \rangle = \langle \varphi(\{\tilde{u}\}(t)), \{w\} \rangle \quad \forall \{w\} \in W. \quad (3.5)$$

273 Again by taking the test vector $\{w\} = \{\phi_k\}$, we have

$$274 \quad \{\phi_k\}^T \boldsymbol{Q} \boldsymbol{\beta}(t) = \{\phi_k\}^T \varphi(\boldsymbol{Q} \boldsymbol{\alpha}(t)).$$

275 Considering all k in $\{1, \dots, K\}$, since $Q = [\{\phi_1\}, \dots, \{\phi_K\}]$ and $Q^T Q = I_K$ we get

$$276 \quad Q^T Q \beta(t) = \beta(t) = Q^T \varphi(Q \alpha(t)).$$

277 It is in the form

$$278 \quad \beta(t) = \varphi_r(\alpha(t)) \quad (3.6)$$

279 with the mapping $\varphi_r : \mathbb{R}^K \rightarrow \mathbb{R}^K$ defined by $\varphi_r(\alpha) = Q^T \varphi(Q \alpha)$. We get a reduced-
 280 order algebraic equilibrium equation. Unfortunately, because of the non-linearities in φ ,
 281 the computation of $\varphi_r(\alpha)$ requires high-dimensional $O(d)$ operations, making this approach
 282 irrelevant from the performance point of view. A possible solution to deal with the non-linear
 283 terms would be to use for example Empirical Interpolation Methods (EIM) (Barrault et al.
 284 2004) but from the algorithm and implementation point of view, this would lead to an
 285 intrusive approach with specific code developments. We here rather adopt a linearization
 286 strategy in the following sense: by derivating (3.6) with respect to time, we get

$$287 \quad \dot{\beta}(t) = \frac{\partial \varphi_r}{\partial \alpha}(\alpha(t)) \dot{\alpha}(t).$$

288 Thanks to the reduced kinematics equation (3.4), we get

$$289 \quad \dot{\beta}(t) = \frac{\partial \varphi_r}{\partial \alpha}(\alpha(t)) \beta(t). \quad (3.7)$$

290 Since φ_r is hard to evaluate, it is even harder to evaluate its differential. But the differential
 291 $\frac{\partial \varphi_r}{\partial \alpha}(\alpha(t))$ can be approximated itself, or replaced by some matrix $A(t)$. Then we get a ROM
 292 structure (ROM prototype) in the form

$$293 \quad \dot{\alpha} = \beta(t), \quad (3.8)$$

$$294 \quad \dot{\beta}(t) = A(t) \beta(t). \quad (3.9)$$

296 The differential system (3.8)-(3.9) is linear with variable coefficient matrix $A(t) \in \mathcal{M}_K(\mathbb{R})$.
 297 It can be written in matrix form

$$298 \quad \frac{d}{dt} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \underbrace{\begin{pmatrix} [0] & I_K \\ [0] & A(t) \end{pmatrix}}_{=A(t)} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}. \quad (3.10)$$

299 The spectral properties of the differential system (3.10) are related to the spectral properties
 300 of matrix $A(t)$. In particular, if all the (complex) eigenvalues $\lambda_k(t)$ of $A(t)$ are such that
 301 $\text{Re}(\lambda_k(t)) < 0$ for all k (uniformly distributed in time), then the system is dissipative.

302 3.3. Nonintrusive approach, SVD decomposition and POD modes

303 One of the requirements of this work is to achieve a non-intrusive reduced-order model,
 304 meaning that the effective implementation of the ROM does not involve tedious low-level
 305 code development into the FOM code. For that, a data-based approach is adopted: from
 306 the FOM code, it is possible to compute FOM solutions ($\{u\}^n, \{v\}^n$) at discrete times t^n ,
 307 $n = 0, \dots, N$ ($t^N = N \Delta t = T$), then store some snapshot solutions (called snapshots) into
 308 a database for data analysis and later design of a ROM. Proper Orthogonal Decomposition
 309 (POD) (Berkooz et al. 1993) is today a well-known dimensionality reduction approach to
 310 determine the principal components from solutions of partial differential equations. The
 311 Sirovich's snapshot variant approach (Sirovich 1987) is based on snapshot solutions from a
 312 FOM to get *a posteriori* empirical POD modes $\{\varphi_k\}$. For the sake of simplicity, assume that
 313 the snapshot solutions are all the discrete FOM solution at simulation instants. Applying a

314 singular value decomposition (SVD) to the displacement snapshot matrix

$$315 \quad \mathbb{S}^u = [\mathbf{u}^1, \mathbf{u}^2, \dots, \mathbf{u}^N],$$

316 of size $d \times N$, we get the SVD decomposition

$$317 \quad \mathbb{S}^u = U\Sigma V^T \quad (3.11)$$

318 with orthogonal matrices $U \in \mathcal{M}_d(\mathbb{R})$, $V \in \mathcal{M}_N(\mathbb{R})$ and the singular value matrix $\Sigma =$
 319 $\text{diag}(\sigma_k) \in \mathcal{M}_{d \times N}(\mathbb{R})$, with $\sigma_k \geq 0$ for all k organized in decreasing order: $\sigma_1 \geq \sigma_2 \geq$
 320 $\dots \geq \sigma_{\min(d,N)} \geq 0$. From SVD theory, for a given accuracy threshold $\varepsilon > 0$, the truncation
 321 rank $K = K(\varepsilon)$ is computed as the smallest integer such that the inequality

$$322 \quad \frac{\sum_{k=K+1}^{\min(d,N)} \sigma_k^2}{\sum_{k=1}^{\min(d,N)} \sigma_k^2} \leq \varepsilon \quad (3.12)$$

323 holds (Shawe-Taylor & Cristianini 2004). Proceeding like that, it is shown that the relative
 324 orthogonal projection error of the snapshots $\{v\}^n$ onto the linear subspace W spanned by the
 325 K first eigenvectors of U is controlled by ε . Denoting π^W the linear orthogonal projection
 326 operator over W , we have:

$$327 \quad \sum_{n=1}^N \|\{v\}^n - \pi^W \{v\}^n\|^2 \leq \varepsilon \sum_{n=1}^N \|\{v\}^n\|^2.$$

328 The matrix Q is obtained as the restriction of U to its K first columns.

329 3.4. Data-driven identification of coefficient matrix

330 The system (3.8)-(3.9) is still not closed since the coefficient matrices $A(t)$ are unknowns.
 331 From FOM data, one can try to identify the matrices by minimizing some residual function
 332 that measures the model discrepancy. The simplest linear model corresponds to the case
 333 where $A(t)$ is searched as a time-constant matrix A . In this case, equation (3.9) becomes
 334 $\dot{\beta}(t) = A\beta(t)$. This is the scope of this article. From the time continuous problem, one could
 335 determine the matrix A by minimizing the least square functional

$$336 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \int_0^T \|\dot{\beta}(t) - A\beta(t)\|^2 dt.$$

337 But practically, we only have velocity snapshot data at discrete times and we do not have
 338 access to the time derivatives of the velocity fields. So the following numerical procedure
 339 is adopted: from the velocity snapshot matrix $\mathbb{S}^v = [\{v\}^1, \dots, \{v\}^N]$, we compute first the
 340 reduced snapshots variables:

$$341 \quad \beta^n = Q \{v\}^n, \quad n = 1, \dots, N.$$

342 Next, we determine a matrix A that minimizes the least square cost function:

$$343 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \sum_{n=1}^{N-1} \left\| \frac{\beta^{n+1} - \beta^n}{\Delta t} - A\beta^n \right\|^2 \quad (3.13)$$

344 In (3.13), the finite difference $\frac{\beta^{n+1} - \beta^n}{\Delta t}$ is a first-order approximation (in Δt) of $\dot{\beta}$ at time
 345 t^n . In appendix A, we provide a mathematical analysis of the effect of time discretization

346 in (3.13) about the impact on the stability of the resulting identified differential system
347 compared to the initial one.

348 The minimization problem (3.13) can be written in condensed matrix form

$$349 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \|\mathbb{Y} - A\mathbb{X}\|_F^2 \quad (3.14)$$

350 with the two data matrices

$$351 \quad \mathbb{X} = [\boldsymbol{\beta}^1, \boldsymbol{\beta}^2, \dots, \boldsymbol{\beta}^{N-1}], \quad \mathbb{Y} = \left[\frac{\boldsymbol{\beta}^2 - \boldsymbol{\beta}^1}{\Delta t}, \dots, \frac{\boldsymbol{\beta}^N - \boldsymbol{\beta}^{N-1}}{\Delta t} \right]. \quad (3.15)$$

352 Because \mathbb{X} and \mathbb{Y} store reduced variables (of size K), for a sufficient number of discrete
353 snapshot times, these two matrices are horizontal ones. We will assume that the rank of \mathbb{X}
354 is always maximal, i.e. equal to K . The least-square solution A of (3.14) is then given by

$$355 \quad A = \mathbb{Y}\mathbb{X}^\dagger \quad (3.16)$$

356 where $\mathbb{X}^\dagger = \mathbb{X}^T(\mathbb{X}\mathbb{X}^T)^{-1}$ is the Moore-Penrose pseudo-inverse matrix of \mathbb{X} . This least
357 square approach has close connections with SVD-based Dynamic Mode Decomposition
358 (DMD) (Schmid 2010; Kutz et al. 2016).

359 3.5. Tikhonov least-square regularized formulation

360 From standard spectral theory arguments, it is expected that the POD coefficients rapidly
361 decay when k increases as soon as both displacement and velocity fields are smooth enough.
362 A possible side effect is the bad condition number of the matrix \mathbb{X} , since the last rows of \mathbb{X}
363 have small coefficients (thus leading to row vectors close to zero 'at the scale' of the first
364 row of \mathbb{X}). Even if the solution A in (3.16) always exists, the solution may be sensitive to
365 perturbations, noise or round-off errors. In order to get a robust identification approach, one
366 can regularize the least-square problem (3.14) by adding a Tikhonov regularization term (see
367 e.g. (Aster et al. 2019))

$$368 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \|\mathbb{Y} - A\mathbb{X}\|_F^2 + \frac{\mu}{2} \|\mathbb{X}\|_F^2 \|A\|_F^2 \quad (3.17)$$

369 where the scalar $\mu > 0$ is the regularization coefficient. The factor $\|\mathbb{X}\|_F^2$ in the regularization
370 term has been added for scaling purposes. The solution A_μ of (3.17) is given by

$$371 \quad A_\mu = \mathbb{Y}\mathbb{X}^T \left(\mathbb{X}\mathbb{X}^T + \mu \|\mathbb{X}\|_F^2 I_K \right)^{-1}. \quad (3.18)$$

372 Choice of optimal regularization coefficient

373 Of course, the solution matrix A_μ depends on the regularization coefficient μ and one can
374 ask what is the optimal choice for μ . There is a trade-off between the approximation quality
375 measured by the residual $\|\mathbb{Y} - A_\mu\mathbb{X}\|_F$ and the norm solution $\|A_\mu\|_F$. The minimization
376 of $\|A_\mu\|_F$ should ensure that unneeded features will not appear in the regularized solution.
377 When plotted on the log-log scale, the curve of optimal values $\mu \mapsto \|A_\mu\|_F$ versus the
378 residual $\mu \mapsto \|\mathbb{Y} - A_\mu\mathbb{X}\|_F$ often takes on a characteristic L shape (Aster et al. 2019). A
379 design of experiment with the test of different values of μ (starting say from 10^{-12} to 10^{-3})
380 generally allow to find quasi-optimal values of μ located at the corner of the L-curve, thus
381 providing a good trade-off between the two criteria.

3.6. Reduced-order continuous dynamical system

382 Once the matrix A_μ has been determined, we get the reduced-order continuous dynamical
383 system
384

$$385 \quad \dot{\alpha} = \beta, \quad (3.19)$$

$$386 \quad \dot{\beta} = A_\mu \beta \quad (3.20)$$

388 with initial conditions $\alpha(0) = \mathbf{0}$, $\mathbf{v}(0) = Q^T \varphi(\{0\})$. At any time t , one can go back to the high-
389 dimensional physical space using the POD modes: $\{u\}(t) = Q\alpha(t)$, $\{x\}(t) = \{X\} + \{u\}(t)$,
390 $\{v\}(t) = Q\beta(t)$. As already mentioned, the system can be written in condensed matrix form

$$391 \quad \dot{\mathbf{w}} = \mathbb{A}_\mu \mathbf{w} \quad (3.21)$$

392 where $\mathbf{w}(t) = (\alpha(t), \beta(t))^T$ and $\mathbb{A}_\mu = \begin{pmatrix} [0]_K & I_K \\ [0]_K & A_\mu \end{pmatrix}$.

393 The exact analytical solution of (3.21) is

$$394 \quad \mathbf{w}(t) = \exp(\mathbb{A}_\mu t) \mathbf{w}(0). \quad (3.22)$$

395 The stability of the differential system depends on the spectral structure of \mathbb{A}_μ , or equivalently
396 on the spectrum of A_μ . Because of the stability of the fluid-capsule coupled system and from
397 accurate solutions of the FOM solver, one can hope that the solution A_μ of the least-square
398 identification problem has the expected spectral properties. This will be studied and discussed
399 in the numerical experimentation section. From the kinetic energy point of view, it is shown
400 in appendix B that the stability of the kinetic energy is linked to the property of the (real)
401 spectrum of the symmetric matrix $(A_\mu + A_\mu^T)/2$.

402 *Model consistency with steady states*

403 A steady state in our context is defined by a capsule that reaches a constant velocity $\{v\}_\infty$,
404 so that the motion becomes a translation flow in time in the direction $\{v\}_\infty$. From (3.1),
405 this shows that $\beta(t)$ also reaches a constant vector β_∞ , and $\dot{\beta} = 0$ at steady state. As a
406 consequence, from (3.20), we get $A_\mu \beta_\infty = 0$, meaning that 0 is an eigenvalue of A_μ with β_∞
407 as eigenvector. As a conclusion, the matrix A_μ must have zero in its spectrum in order to be
408 consistent with the existence of steady states.

409 3.7. Reduced-order discrete dynamical system

410 Of course, it is also possible to derive a discrete dynamical system from the continuous one
411 by using a standard time advance scheme. For example the explicit forward Euler scheme
412 with a constant time step Δt gives

$$413 \quad \alpha^{n+1} = \alpha^n + \Delta t \beta^n, \quad (3.23)$$

$$414 \quad \beta^{n+1} = \beta^n + \Delta t A_\mu \beta^n. \quad (3.24)$$

416 By multiplying (3.23) by Q we get the space-time approximate solution

$$417 \quad \{u\}^{n+1} = \{u\}^n + \Delta t \{v\}^n,$$

418 so the ROM model is completely consistent with the kinematics equation. Stability properties
419 of the discrete system are linked to the spectral properties of the matrix

$$420 \quad A_\mu^\Delta = \begin{pmatrix} I_K & \Delta t I_K \\ [0]_K & (I_K + \Delta t A_\mu) \end{pmatrix}$$

421 For unconditional stability in time, it is required for the eigenvalues of $I_K + \Delta t A_\mu$ to stay in
422 the unit disk of the complex plane.

423 More generally, it is possible to use any other time advance scheme, according to the
424 expected order of accuracy or stability domain.

425 3.8. Accuracy criteria and similarity distances between ROM and FOM solutions

426 In order to quantify the error induced by approximations, we introduce 3 accuracy criteria.
427 The first accuracy criterion is the relative information content (RIC), defined by

$$428 \quad \text{RIC}(K) = \frac{\sum_{k=K+1}^{\min(d,N)} \sigma_k^2}{\sum_{k=1}^{\min(d,N)} \sigma_k^2},$$

429 quantifies the relative amount of neglected information when truncating the number of modes
430 at rank K . The truncation rank is determined such that the RIC is inferior to the accuracy
431 threshold ε . The accuracy threshold ε is fixed to 10^{-6} .

432 The second accuracy criterion is the relative time residual \mathcal{R} . It quantifies the relative error
433 induced by the minimization of the least square cost function (3.13) using A_μ . It is given by

$$434 \quad \mathcal{R}(j) = \frac{\|A_\mu \mathbb{X}_j - \mathbb{Y}_j\|^2}{\|\mathbb{Y}_j\|^2}$$

435 where \mathbb{X}_j represents the j^{th} column of \mathbb{X} and \mathbb{Y}_j the j^{th} column of \mathbb{Y} . The index j is thus
436 linked to the snapshots ($j \in \{1, \dots, N\}$). To better draw a parallel between the evolution of
437 this parameter and the capsule dynamics, this parameter will be represented as a function of
438 the non-dimensional time Vt/ℓ hereafter.

439 The third accuracy criteria $\varepsilon_{\text{Shape}}(Vt/\ell)$ measures the difference between the 3D reference
440 capsule shape given by the FOM (\mathcal{S}_{FOM}) and the 3D shape predicted by the ROM (\mathcal{S}_{ROM}). It
441 is defined at a given non-dimensional time Vt/ℓ as the ratio between the modified Hausdorff
442 distance (MHD) computed between \mathcal{S}_{FOM} and \mathcal{S}_{ROM} and non-dimensionalized by ℓ

$$443 \quad \varepsilon_{\text{Shape}}(Vt/\ell) = \frac{\text{MHD}(\mathcal{S}_{\text{FOM}}(Vt/\ell), \mathcal{S}_{\text{ROM}}(Vt/\ell))}{\ell}$$

444 The modified Hausdorff distance is the maximum value of the mean distance between \mathcal{S}_{FOM}
445 and \mathcal{S}_{ROM} and the mean distance between \mathcal{S}_{ROM} and \mathcal{S}_{FOM} (Dubuisson & Jain 1994).

446 4. Numerical experimentation on a given configuration

447 The method is first applied to a given configuration, in order to set the model parameters
448 and to study its stability and precision. We consider the dynamics of an initially spherical
449 capsule flowing in a microchannel when $Ca = 0.13$ and $a/\ell = 0.8$. The time step between
450 each snapshot Δt equals to 0.04. The dynamics predicted by the FOM is illustrated in Fig. 3
451 up to a non-dimensional time $VT/\ell = 10$. As the capsule flows, its membrane is gradually
452 deformed by the hydrodynamic forces inside the channel during a temporary time until a
453 steady state is reached. We assume that the capsule has reached its steady-state shape, when
454 the surface area of the capsule varies by less than $5 \times 10^{-4} \times (4\pi a^2)$ over a non-dimensional
455 time $Vt/\ell = 1$. For ($Ca = 0.13$, $a/\ell = 0.8$), the steady state is reached at $VT_{SS}/\ell = 6.2$ and
456 is characterized by a parachute capsule shape (Figure 3).

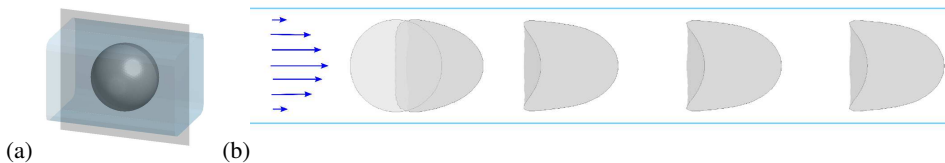


Figure 3: Dynamics of a microcapsule flowing in a microchannel with a square cross-section predicted by FOM in the vertical cutting plane represented in grey in (a). The in-plane capsule profiles are shown for $Ca = 0.13$ and $a/\ell = 0.8$ at the non-dimensional times $Vt/\ell = 0, 0.4, 2, 4, 6$ in (b). The horizontal lines on (b) represent the channel borders. The capsule will always be represented flowing from left to right.

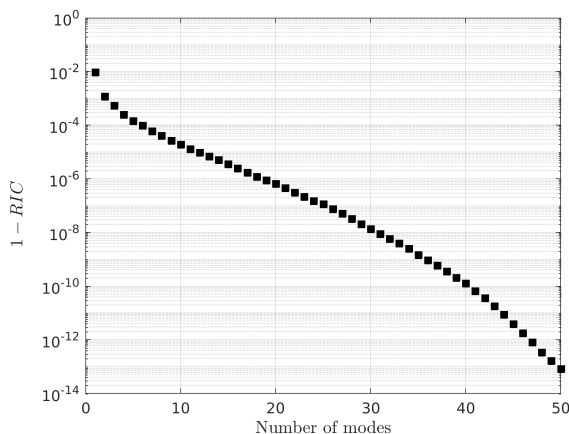


Figure 4: Evolution of the relative amount of neglected information 1-RIC, as a function of the number of modes ($Ca = 0.13, a/\ell = 0.8$).

457

4.1. Proper orthogonal decomposition, truncation and modes

458 The singular value decomposition is first applied to the displacement snapshot matrix. To
 459 determine the truncation rank, the evolution of 1- RIC is illustrated in Figure 4 as a function
 460 of number of modes considered. The RIC is about 1% only with one mode. The more modes
 461 is kept, the less information is neglected. In the following, we fix the number of modes to 20.
 462 The accuracy threshold ε is thus equal to 10^{-6} .

463 The modes are determined from the displacement snapshot matrix. They are added to
 464 the sphere of radius 1 and amplified by a factor 2 to be visualized. The first six modes are
 465 represented in Figure 5 for ($Ca = 0.13, a/\ell = 0.8$).

466 The first six modes are mostly dedicated to change the shape of the rear of the capsule.
 467 The following modes appear to become noisy (not shown). However, these modes are not
 468 negligible, if one wants to get an accuracy of 10^{-6} .

469

4.2. Dynamic Mode Decomposition: empirical regularization

470 Before determining the matrix A , we check the condition number of the matrices \mathbb{X} and
 471 $\mathbb{X}\mathbb{X}^T$. They are respectively equal to 6.5×10^4 and 4.3×10^9 . The condition numbers of these
 472 matrices are very high and the matrix A , determined by solving (3.16), may be sensitive to
 473 perturbations or noise. To improve the robustness, a Tikhonov regularization is applied to
 474 solve the least-square problem (3.13) and the matrix A_μ is computed using (3.18), which
 475 depends on the regularization coefficient μ . To determine the optimal value of μ , the relative
 476 least square error $\|A_\mu \mathbb{X} - \mathbb{Y}\|_F / \|\mathbb{Y}\|_F$ is represented according to the norm solution $\|A_\mu\|_F$

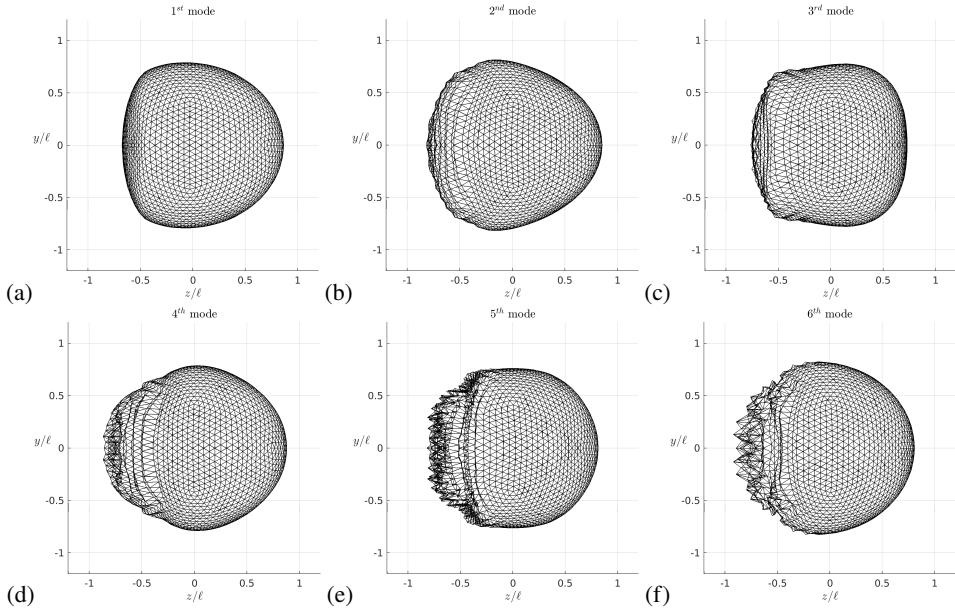


Figure 5: Representation of the first six modes of the capsule dynamics when $a/\ell = 0.80$ and $Ca = 0.13$. To be visualized the modes of displacement were added to the sphere of radius 1 and amplified by a factor 2.

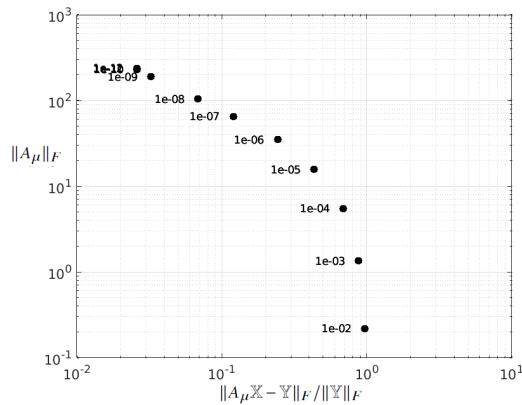


Figure 6: Evolution of the norm solution $\|A_\mu\|_F$ as a function of the least square error $\|A_\mu \mathbb{X} - \mathbb{Y}\|_F / \|\mathbb{Y}\|_F$ when the number of modes is fixed to 20 and ($Ca = 0.13$, $a/\ell = 0.8$).

477 when 20 modes are considered and when μ is varied between 10^{-12} and 10^{-3} (Figure 6).
 478 the least square error $\|A_\mu \mathbb{X} - \mathbb{Y}\|_F$ and the norm solution $\|A_\mu\|_F$ are minimal when $\mu = 10^{-9}$.
 479 In the following, μ is thus fixed to $\mu = 10^{-9}$ and the number of modes to 20.

480 4.3. Validity check of the ROM: spectral study of the resulting matrix

481 In order to detect anomalies, a spectral analysis of the reduced-order model learned by the
 482 DMD method is carried out. The spectrum of the matrix A_μ is represented in Figure 7. All
 483 the eigenvalues λ_k of the matrix A_μ have non-positive real parts. The resulting linear ROM
 484 is thus stable.

485 The temporal evolution of the residual \mathcal{R} (Figure 8) shows that the error is less than

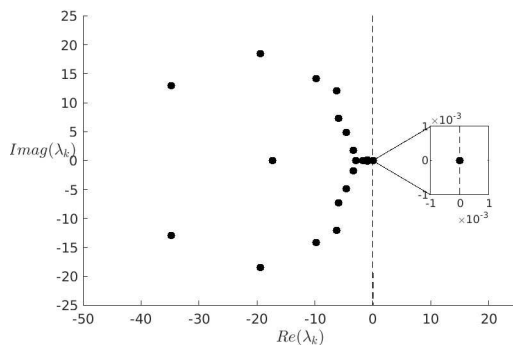


Figure 7: Eigenvalues λ_k of A_μ ($Ca = 0.13$, $a/\ell = 0.8$, 20 modes, $\mu = 10^{-9}$). Note that the maximum real part of the eigenvalues is exactly equal to zero.

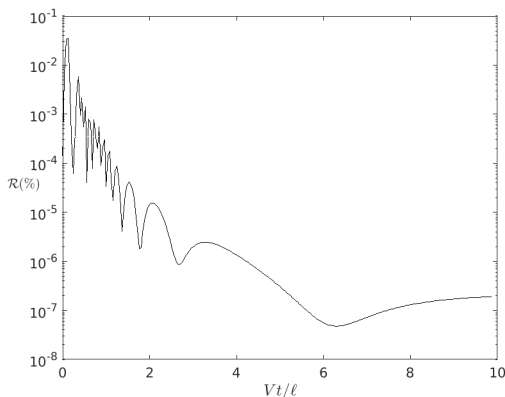


Figure 8: Temporal evolution of the normalized time residual with $Ca = 0.13$, $a/\ell = 0.8$, 20 modes and $\mu = 10^{-9}$.

486 0.7%. The maximal value is reached at the beginning of the simulation ($Vt/\ell < 0.3$) and \mathcal{R}
 487 decreases afterwards. When $Vt/\ell \lesssim 6$, i.e. before the capsule has reached its steady state,
 488 high frequency oscillations are observed. This probably means that a high frequency mode
 489 is neglected, even if 20 modes are considered. For $Vt/\ell > 6$, ε_{ROM} is of order 10^{-9} . The
 490 stationary state is thus well predicted by the model and the error during the transient stage is
 491 more than acceptable.

492

4.4. ROM online stage and accuracy assessment

493 The displacement of all the nodes of the capsule mesh estimated by the ROM is then added
 494 to the corresponding node of the sphere of radius 1 to visualize the temporal evolution of the
 495 capsule shape in three dimensions. Figure 9 shows the capsule dynamics for the reference case
 496 ($Ca = 0.13$, $a/\ell = 0.8$). The ROM allows us to reproduce the capsule deformation from the
 497 initial state up to the parachute-shaped steady state. For the FOM and the ROM, the capsule
 498 profile is then determined in the cutting plane passing through the middle of the microchannel.
 499 Figure 10 shows that the two capsule profiles perfectly overlap at $Vt/\ell = 0, 0.4, 2, 4, 6$. The
 500 temporal evolution of ε_{Shape} is shown in Figure 11a. The maximum value of the error

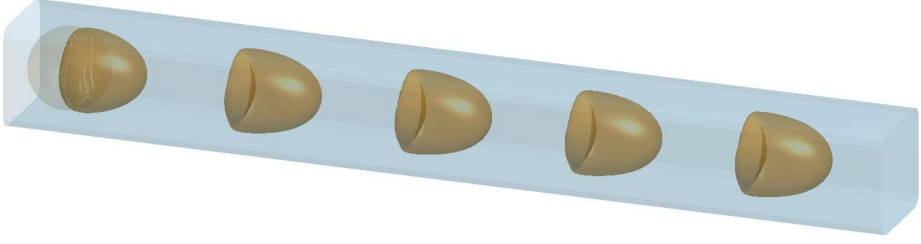


Figure 9: Dynamics of a microcapsule flowing in microchannel with a square cross-section predicted by ROM at the non-dimensional time $Vt/\ell = 0.4, 2.8, 5.2, 7.6, 10$ with $Ca = 0.13$, $a/\ell = 0.8$, 20 modes and $\mu = 10^{-9}$. The initial spherical capsule is shown on the left by transparency.

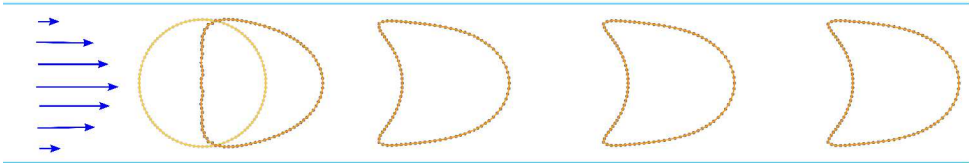


Figure 10: Comparison of the capsule contours given by the FOM (dotted line) and estimated by the ROM (orange line). The capsule is shown for $(Ca = 0.13, a/\ell = 0.8)$ at the non-dimensional time $Vt/\ell = 0, 0.4, 2, 4, 6$. The horizontal lines represent the channel borders. The number of modes is fixed to 20 and $\mu = 10^{-9}$.

501 committed on the 3D shape $\varepsilon_{\text{Shape}}$ equals to 0.004%. The error on the capsule shape $\varepsilon_{\text{Shape}}$ is
 502 thus negligible. The deformation of the capsule from its initially spherical shape to its steady
 503 state over an non-dimensional time $Vt/\ell = 10$ can thus be estimated very precisely with the
 504 developed reduced-order model.

505 The DMD method predicts the capsule displacement at time t^{n+1} from that at time t^n . The
 506 model has been constructed until now by considering the dynamics of the capsule over a
 507 non-dimensional time Vt/ℓ of 10.

508 In order to study the sensitivity of the ROM on the learning time VT_L/ℓ , i.e. the non-
 509 dimensional time over which the model is trained, we modify it with values between 2 and
 510 8, knowing that the time to reach the steady state is in this case $VT_{SS}/\ell = 6.2$. We estimate
 511 the capsule dynamics using the ROM model up to a non-dimensional time Vt/ℓ of 10. The
 512 number of modes is always equal to 20 and $\mu = 10^{-9}$. The comparison of the estimated
 513 shape at $Vt/\ell = 10$ with the one simulated with the FOM (Figure 11a) shows that $VT_L/\ell \geq 4$
 514 is sufficient to predict very well the capsule dynamics. The Figure 11b confirms that the
 515 error on the capsule shape is negligible when $VT_L/\ell \geq 4$. It is interesting that the ROM
 516 model could predict the steady state even when $T_L < T_{SS}$. This could be due to the fact that
 517 the maximum real part of the eigenvalues is exactly equal to zero from $VT_L/\ell \geq 4$. The
 518 maximum real part of the eigenvalues is negative and close to zero for $VT_L/\ell = 2$. Figure 11c
 519 shows that, in the worst case ($VT_L/\ell = 2$), the error on the capsule shape increases with time
 520 but reaches a plateau from a time Vt/ℓ of 8. The system is thus stable without exponential
 521 drift as proven by the negative value of the maximum real eigenvalue. In the zoom insert, the
 522 error also increases for the other learning times but remains very small (below 0.2%).

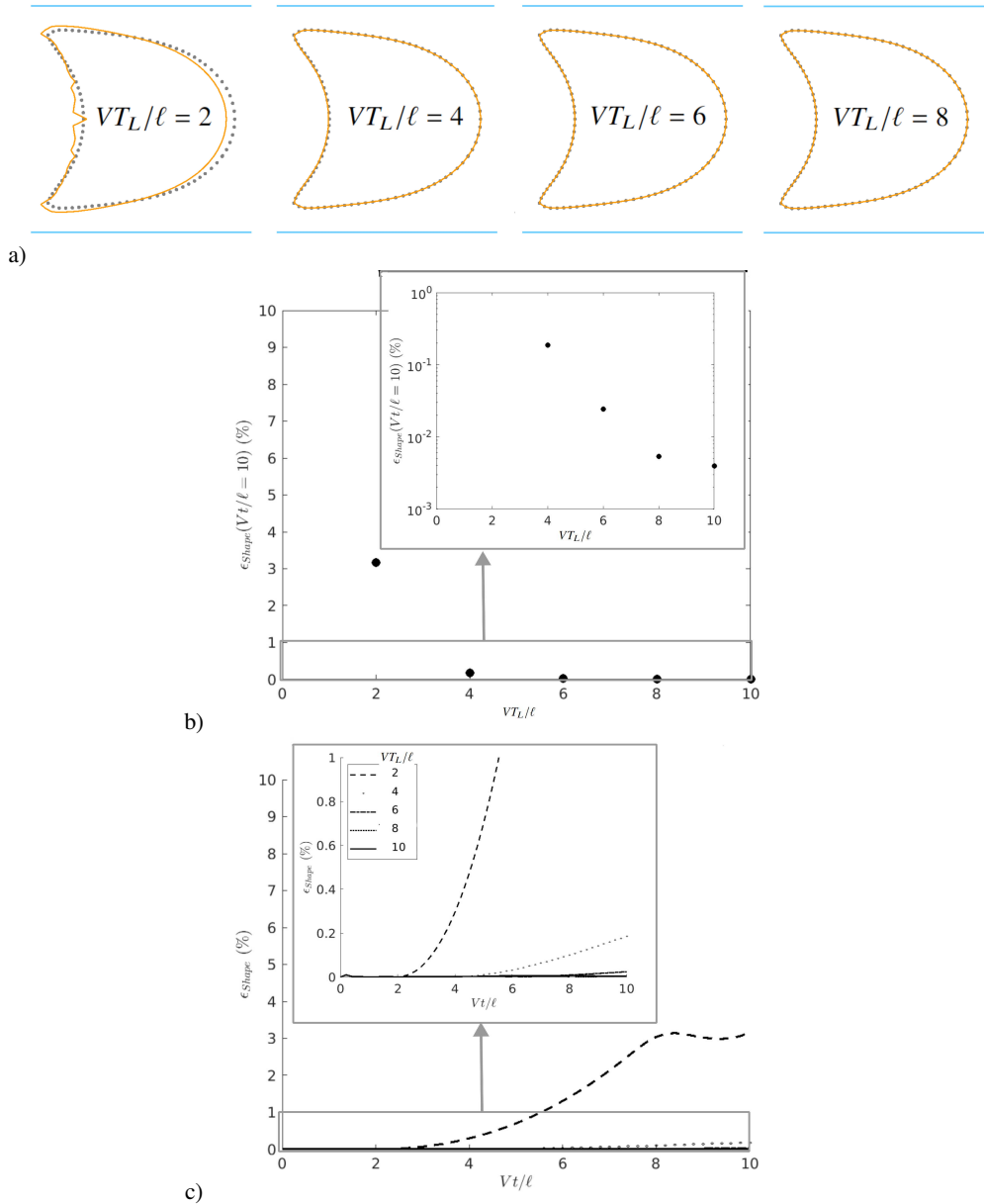


Figure 11: a) Comparison of the capsule contours given by the FOM (dotted line) and estimated by the ROM (orange line) for the different learning times VT_L/ℓ . b) Evolution of ϵ_{Shape} measured at $Vt/\ell = 10$ as a function of the learning time VT_L/ℓ . c) Influence of the learning time VT_L/ℓ on the temporal evolution of the error on the capsule shape ϵ_{Shape} . The error during the learning time is shown in solid line. For this case, the parameters are 20 modes, $\mu = 10^{-9}$, $Ca = 0.13$ and $a/\ell = 0.8$.

523 5. Space-time ROM accuracy assessment over the full parameter sample set

524 The capillary number Ca and the size ratio a/ℓ are now considered as variable parameters.
 525 A database of 119 simulations of the deformation of an initially spherical capsule in a
 526 microchannel has been generated using the FOM with the same time step and mesh size as in

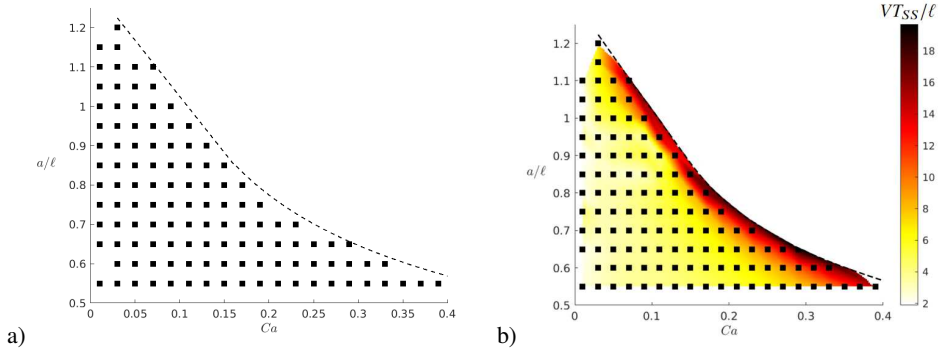


Figure 12: a) Values of Ca and a/ℓ included in the training database. b) Evolution of the time VT_{SS}/ℓ needed to reach the steady state, on the training database. The dotted line delimits the domain where a steady-state capsule deformation exists for capsules following the neo-Hookean law.

527 section 4. Figure 12a shows the different values of Ca and a/ℓ for which the simulations have
 528 been computed to create the training database. When the capsule initial radius is close to
 529 or larger than the microchannel cross-dimension ($a/\ell \geq 0.90$), the capsule is pre-deformed
 530 into a prolate spheroid to fit in the channel. For a given a/ℓ , a limit value of Ca exists
 531 beyond which a capsule does not reach a steady-state (Figure 12). This is due to the softening
 532 behavior of the neo-Hookean law.

533 For the following, we have considered a learning time $VT_L/\ell = 10$. The evolution of the
 534 time VT_{SS}/ℓ needed to reach the steady state is illustrated in Figure 12b on the whole training
 535 database. The steady state is reached on average at a time VT_{SS}/ℓ of 6.2. However, we notice
 536 that for the cases close to the steady state limit, VT_{SS}/ℓ increases and exceeds the considered
 537 learning time.

538 For all the couples $(Ca, a/\ell)$ of the training database, the capsule shape is reconstructed
 539 from the ROM results at given non-dimensional times and compared to the shape predicted
 540 by the FOM at the same non-dimensional time. The evolution of the error committed
 541 on the capsule shape ε_{Shape} on the full database is illustrated in Figure 13 at $Vt/\ell =$
 542 0, 0.4, 1, 2, 5, 10. ε_{Shape} is null at $Vt/\ell = 0$. The ROM is therefore able to predict the initial
 543 capsule shape correctly, whether it is spherical or slightly ellipsoidal. Until $Vt/\ell \leq 2$, ε_{Shape}
 544 essentially remains zero on the majority of the database. Otherwise, it is equal to 0.15% at
 545 maximum. At $Vt/\ell = 5$ and 10, the error ε_{Shape} slightly increases for most of the couples
 546 $(Ca, a/\ell)$ of the database. It remains fully acceptable since it is equal to 0.35% at maximum.
 547 When considering 20 modes and $\mu = 10^{-9}$, the developed ROM allows us to estimate with
 548 great precision the dynamics of an initially spherical capsule in a microchannel with a square
 549 cross-section.

550 To respect the stability condition (see Equation 2.10), the time step imposed to simulate
 551 the capsule dynamics with the FOM decreases, when the Ca decreases. The lower the Ca ,
 552 the longer the simulation lasts (Figure 2). The time needed to calculate the capsule shape and
 553 write the results was estimated on the same workstation used to simulate and generate the
 554 result files with the FOM (2-CPU Intel® Xeon® Gold 6130, 2.1 GHz). The speedup is the
 555 ratio between the FOM runtime and the ROM runtime. Its evolution according to the FOM
 556 time step is illustrated in Figure 14. It was estimated from the ROM and FOM simulation
 557 time obtained when $a/\ell = 0.7$. The speedup varies between 52106 for a FOM time step of
 558 10^{-4} (i.e for the lowest value of Ca tested) and 4200 for 5×10^{-4} (i.e $Ca \geq 0.05$). It is thus

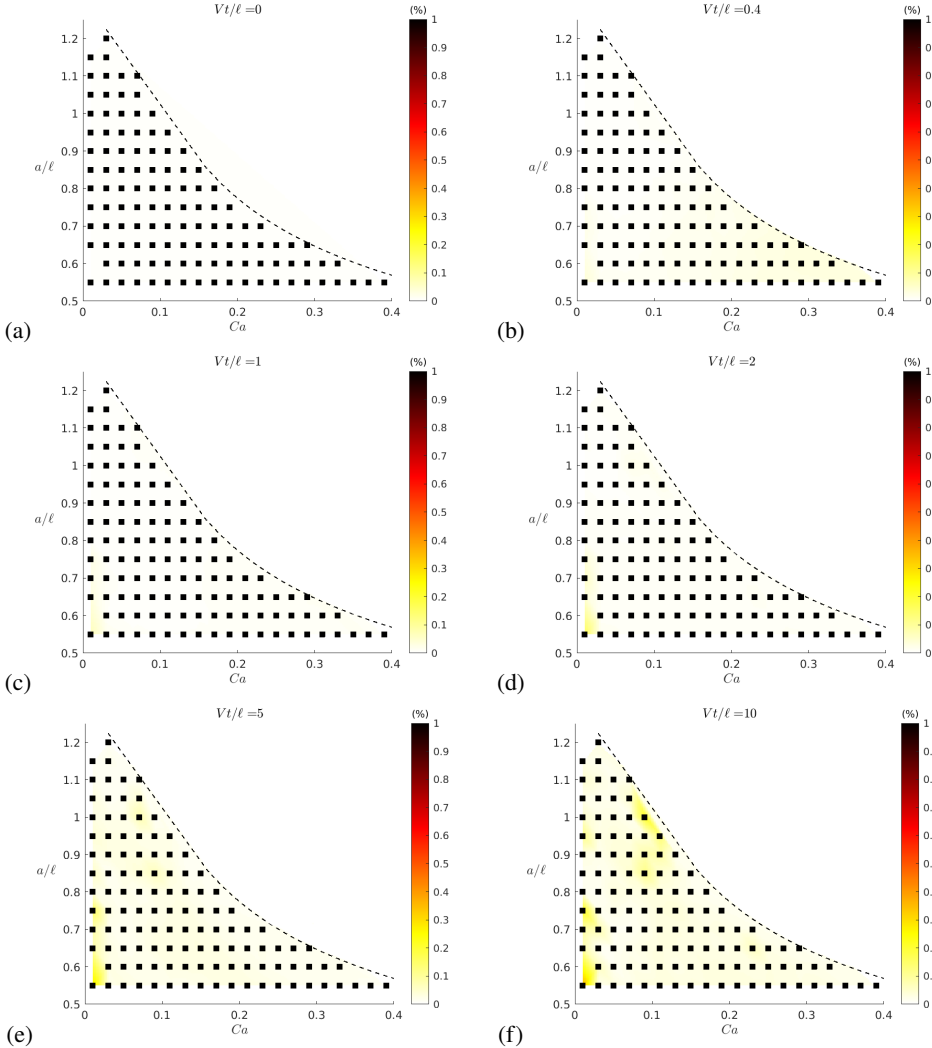


Figure 13: Heat maps of ϵ_{Shape} on the training database as a function of Ca and a/ℓ at (a) $\dot{\gamma}t=0$, (b) 0.4, (c) 1, (d) 2, (e) 5, (f) 10 (obtained with 20 modes and $\mu = 10^{-9}$). The dotted line delimits the domain where a steady-state capsule deformation exists.

559 possible to estimate the capsule dynamics very precisely with the developed ROM, while
 560 considerably reducing the computational time.

561 Another significant advantage is the gain in storage of the simulation results. By storing
 562 only the reduced variables α , β , the modes $\{\phi_k\}$ and the initial position of the nodes of each
 563 couple $\theta = (Ca, a/\ell)$, the training database is reduced from 1.9 GB, when computed with
 564 the FOM, to 0.15 GB with the ROM. It can therefore be more easily shared.

565 6. Full space-time-parameter ROM (for any admissible parameter value)

566

6.1. General methodology

567 It is here again assumed that a training database of N precomputed FOM results is available.
 568 Now we would like to derive a ROM for any parameter couple $\theta = (Ca, a/\ell)$ in the admissible

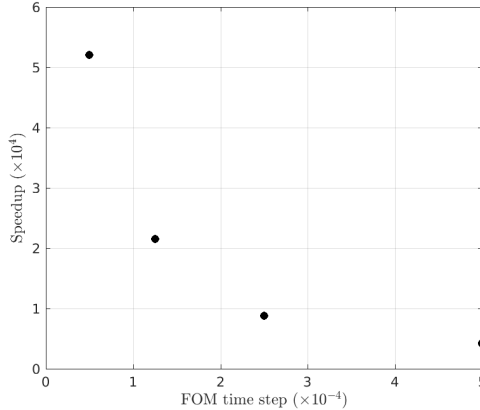


Figure 14: Evolution of the speedup as function to the time step imposed to simulate the capsule dynamics with the FOM ($a/\ell = 0.7$).

569 parameter domain. The proposed space-time-parameter ROM is made of two steps. The first
 570 step consists in predicting the space-time solution $\{\mathbf{u}\}(t; \boldsymbol{\theta})$ by means of a robust interpolation
 571 procedure. The second step consists in deriving a ROM in the form of a low-order dynamical
 572 system by using the predicted solutions of the first step as training data. Then we apply the
 573 former procedure detailed in Section 3. Below we give a detailed explanation of the two
 574 steps.

575 **Step 1: predictor step.** Considering a parameter couple $\boldsymbol{\theta}$, we first search the three
 576 nearest neighbour parameters in the sample set that form a non-degenerate triangle in the
 577 plane ($Ca, a/\ell$). Let us denote them by $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$ and $\boldsymbol{\theta}_3$. We will define a linear operator in
 578 the triangle $(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3)$. For that, let us introduce the barycentric coordinates $(\lambda_1, \lambda_2, \lambda_3)$,
 579 $\lambda \in [0, 1], i = 1, 2, 3$ such that

$$580 \quad \lambda_1 + \lambda_2 + \lambda_3 = 1, \quad (6.1)$$

$$581 \quad \boldsymbol{\theta}_1 \lambda_1 + \boldsymbol{\theta}_2 \lambda_2 + \boldsymbol{\theta}_3 \lambda_3 = \boldsymbol{\theta}. \quad (6.2)$$

583 The 3×3 linear system (6.1),(6.2) is invertible as soon as the triangle $(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3)$ is non-
 584 degenerate. Notice that the λ_i ($i = 1, 2, 3$) are actually functions of $\boldsymbol{\theta}$. Let us now denote
 585 by $\{u_1\}, \{u_2\}$ and $\{u_3\}$ the displacement fields for the parameter vectors $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2$ and $\boldsymbol{\theta}_3$
 586 respectively. Then we can consider the predicted velocity field $\hat{\mathbf{u}}(t; \boldsymbol{\theta})$ defined by

$$587 \quad \{\hat{\mathbf{u}}\}(t, \boldsymbol{\theta}) = \lambda_1 \{u_1\}(t) + \lambda_2 \{u_2\}(t) + \lambda_3 \{u_3\}(t). \quad (6.3)$$

Step 2: low-order dynamical system ROM. Expression (6.3) can be evaluated at
 some discrete instants in order to generate new training data. Then the SVD-DMD ROM
 methodology presented in Section 3 can be applied to these data to get a reduced dynamical
 system in the form

$$\begin{aligned} \dot{\boldsymbol{\alpha}}(\boldsymbol{\theta}) &= \boldsymbol{\beta}(\boldsymbol{\theta}), \\ \dot{\boldsymbol{\beta}}(\boldsymbol{\theta}) &= A_\mu(\boldsymbol{\theta}) \boldsymbol{\beta}(\boldsymbol{\theta}). \end{aligned}$$

588 We also have a matrix $Q(\boldsymbol{\theta})$ of orthogonal POD modes and we can go back to the high-
 589 dimensional physical space by the standard operations

$$590 \quad \{\hat{\mathbf{u}}\}(t, \boldsymbol{\theta}) \approx Q(\boldsymbol{\theta}) \boldsymbol{\alpha}(t, \boldsymbol{\theta}), \quad \{\hat{\mathbf{v}}\}(t, \boldsymbol{\theta}) \approx Q(\boldsymbol{\theta}) \boldsymbol{\beta}(t, \boldsymbol{\theta}). \quad (6.4)$$

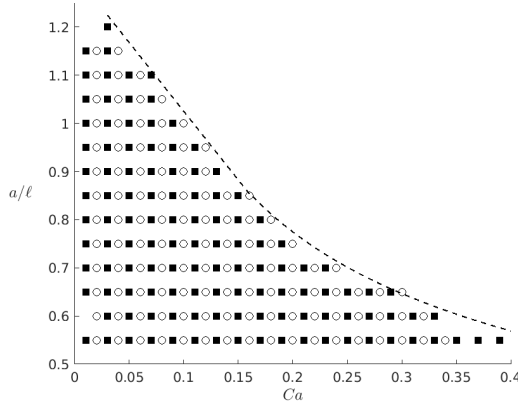


Figure 15: Values of Ca and a/ℓ included in the testing database (open circle). The filled squares represent the cases in the training database. The dotted line delimits the domain where a steady-state capsule deformation exists for capsules following the neo-Hookean law.

591 Notice that the capsule position field $\{x\}(t, \theta)$ is given by

$$592 \quad \{x\}(t; \theta) = \{X\}(\theta) + \{\hat{u}\}(t, \theta)$$

593 with an initial capsule position $\{X\}(\theta)$ that may depend on θ because of the pre-deformation
594 preprocessing if $a/\ell \geq 0.95$.

595 A testing database is created using the FOM as in Section 5 and considering $(Ca, a/\ell)$ -
596 couples which are not in the training database. A set of 110 $(Ca, a/\ell)$ -couples are included
597 in this database (Figure 15). For all the $(Ca, a/\ell)$ -couples of the testing database, the capsule
598 dynamics is interpolated from the dynamics of the 3 closest neighbours at a given non-
599 dimensional time. Capsule shapes obtained by the ROM are compared to the ones predicted
600 by the FOM at the same non-dimensional time. Figure 16 represents the evolution of the error
601 committed on the capsule shape ε_{Shape} on the training database at $Vt/\ell = 0, 0.4, 1, 2, 5, 10$.
602 At initial time, ε_{Shape} is zero. The interpolation method is therefore able to capture the initial
603 capsule shape. When the time increases, ε_{Shape} increases and greater than if we apply directly
604 the POD-DMD method on the FOM results and reconstruct the dynamics. However, ε_{Shape}
605 remains less than 0.3% on the majority of the testing database. It remains fully acceptable.
606 ε_{Shape} is more important near the steady-state limit and when we approach the lowest values
607 of Ca because we are close to the limits of the training base.

608 7. Application of the ROM to a capsule in simple shear flow

609 To prove the generality of the proposed approach, we additionally apply the ROM to a
610 capsule in simple shear flow. This classical case was extensively studied over the past years
611 (Ramanujan & Pozrikidis 1998; Lac & Barthès-Biesel 2005; Li & Sarkar 2008; Walter et al.
612 2010; Foessel et al. 2011; Barthès-Biesel et al. 2010; Dupont et al. 2015). The FOM results
613 of an initially spherical capsule subjected to a shear rate $\dot{\gamma}$ are simulated using the unconfined
614 version of the boundary integral - finite element method presented in section 2 (see
615 Walter et al. (2010) for a detailed description of the method). The time step Δt between
616 each snapshot is equal to 0.04.

617 We first build a ROM model that predicts the capsule dynamics until $\dot{\gamma}t = 10$ with 15
618 modes, a learning time of $\dot{\gamma}T_L = 10$ and $\mu = 10^{-6}$. We retrieve that the initial spherical

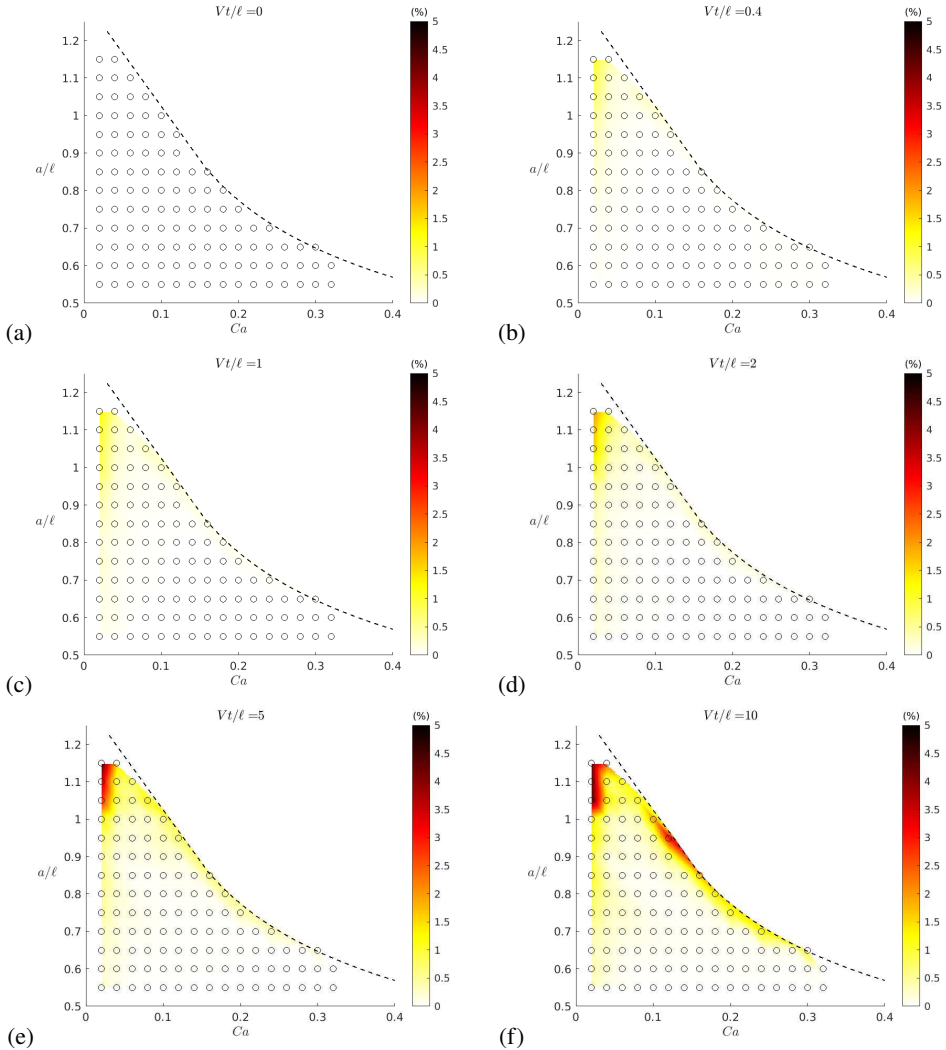


Figure 16: Heat maps of $\varepsilon_{\text{Shape}}$ on the testing database as a function of Ca and a/ℓ at (a) $\dot{\gamma}t=0$, (b) 0.4, (c) 1, (d) 2, (e) 5, (f) 10. The dotted line delimits the domain for which a steady-state capsule deformation exists.

619 capsule elongates under the effect of the external flow in the straining direction and that the
 620 membrane rotates around the deformed shape due to the flow vorticity (Figure 17). The ROM
 621 is thus able to recover the tank-treading motion. A very good agreement between the ROM
 622 and FOM is seen in Figure 18 for the capsule profiles in the shear and perpendicular planes.
 623 Figure 19 shows the evolution of the maximum error on the capsule shape for different values
 624 of Ca . At $Ca = 0.1$, the ROM model predicts well the time evolution of the global capsule
 625 shape but not precisely the wrinkle formation, leading to 2% error on average. But from
 626 $Ca \geq 0.3$, the error is reduced by an order of magnitude and is below 0.2%.

627 We then perform some tests to be sure that the model is able to predict the tank-treading
 628 motion correctly after the learning time. Since the period is equal to 17.6 for $Ca = 0.3$, the
 629 learning time $T_L = 10$ appears to be too short to capture the periodical motion. We consider
 630 a (safe) learning time $T_L = 20$ and increase the number of modes to 60 to capture the

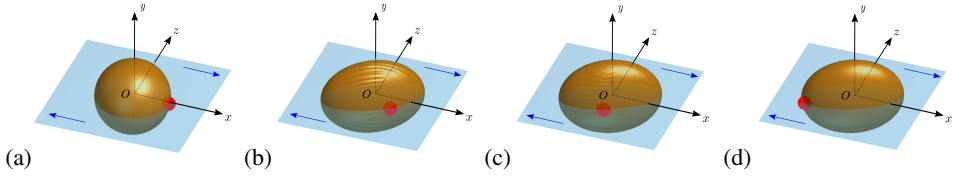


Figure 17: Snapshots of a capsule subjected to a simple shear flow estimated by the ROM ($Ca = 0.3$, 15 modes and $\mu = 10^{-6}$): $\dot{\gamma}t = 0$ (a), 1.6 (b), 4.8 (c), 6.4 (d). A red point is placed on the membrane to visualize the tank-treading motion.

631 Lagrangian motion of the mesh along the capsule (Eulerian) steady shape. This convection-
 632 dominated motion of the capsule is known to be an unfavourable condition for dimensionality
 633 reduction and this is the reason why it is adequate to increase the number of modes. We have
 634 obtained the best tradeoff between accuracy, numerical conditioning and complexity using
 635 60 modes.

636 The error on the 3D shape $\varepsilon_{\text{Shape}}$, represented in Figure 20a, does not exceed 2%. Indeed,
 637 after a quasi-monotonic increase, it reaches a value of 1.7 at the end of the learning time
 638 ($\dot{\gamma}t \leq 20$) and remains almost constant during the extended prediction time ($20 < \dot{\gamma}t \leq 30$).
 639 This is very comforting for long-time stability and accuracy of the simulation. Furthermore,
 640 we study the spectral structure of the matrix A_μ and plot its eigenvalues in the complex
 641 plane in Figure 20b. All the eigenvalues have non-positive real parts showing the asymptotic
 642 stability property of the dynamical system.

643 One may still wonder whether the DMD-ROM model is accurate only for capsule flows that
 644 converge towards a steady state. To answer the question, we have investigated the feasibility
 645 of applying the method to an initially ellipsoidal capsule in simple shear flow. Depending on
 646 the parameters, such a capsule exhibits a variety of dynamical regimes, which are periodical
 647 in many cases (Walter *et al.* 2011; Dupont *et al.* 2013, 2016). We apply the ROM model to
 648 the full dataset of FOM simulations for the same initial capsule. It is thus a case where the
 649 ergodicity hypothesis cannot be applied to improve the filling of the state space (see Tu *et al.*
 650 (2014)).

651 At large Ca , when the capsule exhibits a fluid-like behaviour, a large number of modes
 652 is required to capture the membrane rotation around the deformed shape. When the capsule
 653 behaves like a solid particle at low Ca and exhibits a tumbling motion, it is preferable to
 654 place the capsule within its own reference frame before applying the ROM method. The
 655 error is typically of a few percent and the capsule motion is well reproduced. An example
 656 of the tumbling dynamics predicted by the ROM is compared to the one simulated by the
 657 FOM in Figure 21. The ROM is able to reproduce more complex capsule dynamics (e.g.
 658 with periodical motion) and to capture deformation features including wrinkles, all this with
 659 a speedup of about 35 000.

660 8. Discussion and conclusion

As a summary, in this paper we have considered a θ -parametrized reduced-order model of microcapsule dynamics in the form

$$\begin{aligned}\dot{\alpha}(\theta) &= \beta(\theta), \\ \dot{\beta}(\theta) &= A_\mu(\theta) \beta(\theta).\end{aligned}$$

661 The vector $\theta = (Ca, a/\ell)$ contains the governing parameters, the coefficients $\alpha_k(t, \theta)$ and
 662 $\beta_k(t, \theta)$ are spectral coefficients of POD decomposition for the displacement and velocity

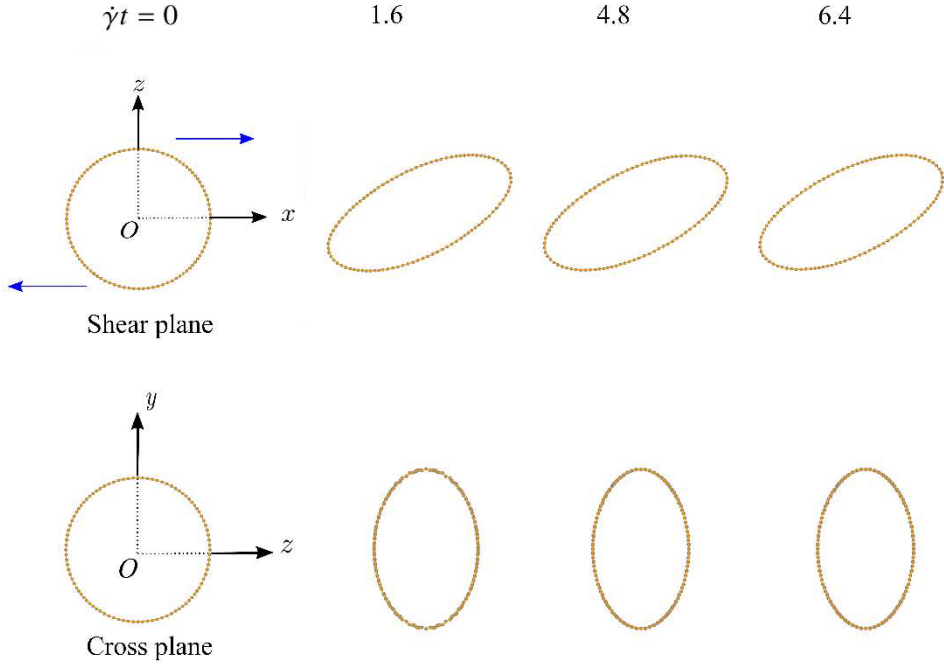


Figure 18: Capsule subjected to a simple shear flow for $Ca = 0.3$: Comparison of the contours in the shear and cross planes given by the FOM (dotted line) and estimated by the ROM (orange line, obtained with 15 modes and $\mu = 10^{-6}$).

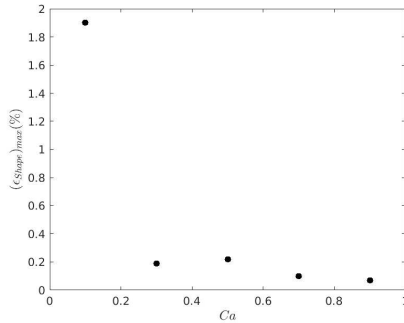


Figure 19: Evolution of the maximum error committed on the shape of a capsule subjected to a simple shear flow as a function of the capillary number Ca (obtained with 15 modes and $\mu = 10^{-6}$). The capsule dynamics was simulated up to a non-dimensional time $\dot{\gamma} = 10$.

663 fields respectively, and the matrix $A_\mu(\theta)$ is identified from data using a dynamic mode
 664 decomposition least-square procedure. We have numerically proven for a broad range of
 665 capillary numbers Ca and size ratios a/ℓ that it is able to capture the dynamics up to the
 666 steady state of a capsule flowing in a channel and its large deformations. As a first approach,
 667 we have presently chosen to use a DMD method that is linear in time to build the ROM
 668 model. Still the ROM model captures spatial non-linearity by means of the POD modes. The
 669 resulting reduced-order model is of great fidelity, weak discrepancies being only observed
 670 in the early transient stage. We have also shown that the learning time need to be larger than

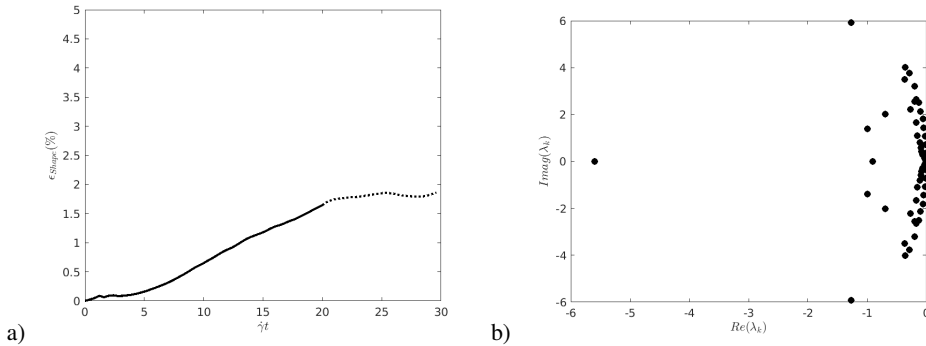


Figure 20: a) Evolution of the error committed on the shape of a capsule subjected to a simple shear flow during the learning time (full line) and the extended prediction time (dotted line). b) Representation of the eigenvalues of A_μ when 60 modes, $\mu = 10^{-6}$ and $Ca = 0.3$ are considered.

671 the transient stage duration and that we can go beyond the FOM time window used for the
672 training of the ROM model.

673 For generalisation, we have computed the capsule dynamics for any parameter set. The
674 generalization algorithm is based on interpolation: we first pre-calculate the ROM dynamic
675 model at a finite number of points in the parameter space domain and determine the α ,
676 β and ϕ_k (and thus the capsule displacement) at these points. For any other value of the
677 parameters, we first predict the time-evolution of the capsule node displacements using a
678 linear interpolation procedure in the parameter space and then build a dynamical system
679 based the DMD methodology. The error is mostly below 0.3% over the entire domain, which
680 proves the precision and utility of the ROM approach.

681 Like any other data-driven model, the model requires a certain number of high-fidelity
682 simulations to provide accurate predictions. By discretizing the parameter space in a regular
683 and homogeneous way (Figure 12), we have not presently tried to optimize the number of
684 FOM simulations. But sampling strategies like the Latin Hypercube Sampling (LHS) exist
685 and result in a net reduction in FOM simulation number. The empirical law, conventional
686 among the data-driven model community, is that one needs between $10 \times D$ and $50 \times D$
687 points, where D is the dimension of the problem ($D = 2$ in our case). This law shows that the
688 number of high-fidelity simulations does not explode with the problem dimension, owing to
689 the linear dependence of the law.

690 The linear differential model is stable as soon as the eigenvalues of A_μ have non-positive
691 real parts, and is consistent with steady states as soon as zero is an eigenvalue. Numerical
692 experiments show that identified matrices A_μ from data have eigenvalues with negative real
693 parts and one of the eigenvalues is very close to zero.

694 As it is often the case with spectral-like methods, there is a trade-off between accuracy
695 and ill-conditioning effects: when a large number of POD modes are used ($K > 20$), the
696 data matrix \mathbb{X} of snapshot POD coefficients is ill-conditioned. For the determination of A_μ ,
697 we have used a Tikhonov regularization in the least square cost function (see (3.17)) in
698 order to have a better conditioned problem and a L -curve procedure to determine the best
699 regularization coefficient μ . Unfortunately we observe some limitations in the accuracy.
700 A perspective would be to use a proximal approach: within an iterative procedure, at

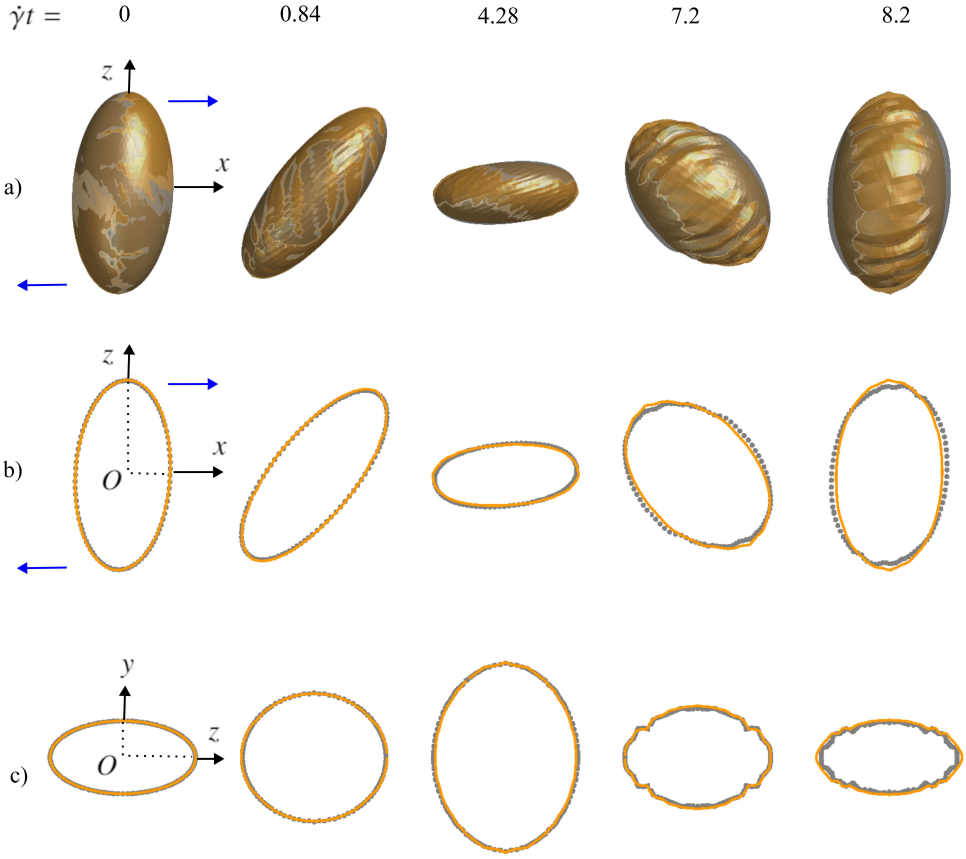


Figure 21: Tumbling motion of a prolate capsule (aspect ratio = 2) subjected to a simple shear flow ($Ca = 0.1$): a) Comparison of the 3D shape given by the FOM (in gray) and estimated by the ROM (in orange, obtained with 50 modes and $\mu = 10^{-6}$). Comparison of the 2D profil b) in the shear plane and c) in the crossed plane. The time step Δt between each snapshot is equal to 0.04.

701 iteration $(p + 1)$, compute the matrix $A_\mu^{(p+1)}$ solution of

$$702 \quad A_\mu^{(p+1)} = \arg \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \|\mathbb{Y} - A\mathbb{X}\|_F^2 + \frac{\mu}{2} \|\mathbb{X}\|_F^2 \|A - A_\mu^{(p)}\|_F^2$$

703 using $A_\mu^{(0)} = 0$. At convergence, one can observe that the regularization term vanishes, so
 704 that one can expect better accuracy with this approach. This will be investigated in a future
 705 work.

706 We have proposed a successful and very efficient ROM for FSI problems. It is an alternative
 707 to the use of HPC. It must be seen as a complimentary (and non-competing) approach to
 708 full-order models, and has many advantages. Among them, one can mention the easiness
 709 in implementation. It leads to a very handy set of ODEs, that are easy to determine from
 710 an algorithmic point of view. Furthermore, the system can be run on any computer. The
 711 size of the matrices is, indeed, reduced from $(3 \times 2562 \text{ nodes} \times 250 \text{ snapshots})$ to about
 712 $(3 \times 2562 \text{ nodes} \times (K + 1))$, where the number of modes is $K = 20$. The computation required

713 time is a few milliseconds for one parameter set. The current speedups are between 5 000 and
 714 52 000, which out-performs any full-order model approach. We believe that this work is an
 715 encouraging milestone to move toward real time simulation of general coupled problems and
 716 to deal with high-level parametric studies, sensitivity analysis, optimization and uncertainty
 717 quantification.

718 The next milestone following this work would be to go toward non-linear differential
 719 dynamical systems as reduced-order models. There is three natural ways for that. The first
 720 one is to use Kernel Dynamic Model Decomposition (KDMD) rather than DMD. But we have
 721 recently shown in De Vuyst *et al.* (2022) that a non-linear low-order dynamical model does
 722 not provide significant improvement. The second one is to use Extended Dynamic Model
 723 Decomposition (EDMD) (Williams *et al.* 2015). The EDMD method adds some suitable
 724 non-linear observables (or features) in the data, so that a linear 'augmented' dynamical
 725 system is searched for. A third option is would be to directly use artificial neural networks
 726 (ANN), in particular recurrent neural networks (RNN) (Trischler & D'Euleuterio 2016). The
 727 RNN training would replace the DMD procedure, and would be trained with the same POD
 728 coefficient matrices \mathbb{X} and \mathbb{Y} . As shown in the recent study by Lin *et al.* (2021), artificial
 729 intelligent may prove to be efficient and precise to predict capsule deformation.

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738 **Author contributions.** A.V.S and F.D.V. created the research plan and formulated the numerical problem.
 739 C.D. implemented the numerical method and performed the tests. All authors contributed to analysing data
 740 and reaching conclusions, and in writing the paper.

741 **Appendix A. Effects of time derivative discretization on matrix estimation**

742 In section 3.4, we explain how to identify the coefficient matrix A from a least square problem
 743 that tries to minimize the squared residual $\int_0^T \|\dot{\boldsymbol{\beta}}(t) - A \boldsymbol{\beta}(t)\|^2 dt$. For practical reasons
 744 and because of a finite number of data, we have to discretize the functional and in particular
 745 the time derivatives by means of finite differences. This section is dedicated to the analysis
 746 of the effect of discretization on the estimation on A , and in particular on the effect on the
 747 spectrum of A and the impact on the stability of the identified model.

748 The notations here are specific to this section. Suppose we have a reference linear dynamical
 749 system whose equations and initial data are respectively

$$750 \quad \dot{\boldsymbol{v}} = A^{ref} \boldsymbol{v}, \quad t \in [0, T], \quad \boldsymbol{v}(0) = \boldsymbol{v}^0 \in \mathbb{R}^K,$$

751 where $A^{ref} \in \mathcal{M}_K(\mathbb{R})$. The solution of the differential problem is given by $\boldsymbol{v}(t) =$
 752 $\exp(A^{ref} t) \boldsymbol{v}^0, t \in [0, T]$. Suppose that we don't know A^{ref} but we have access to the exact
 753 solutions $\boldsymbol{v}^n = \boldsymbol{v}(t^n)$ at discrete times $t^n = n\Delta t, n \in \{0, \dots, N\}$ where with $\Delta t = T/N$. The
 754 $(\boldsymbol{v}^n)_n$ will be used as data for the identification (estimation) of the matrix A^{ref} . Consider

755 the least square minimization problem

$$756 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \sum_{i=0}^{N-1} \left\| \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} - A \mathbf{v}^n \right\|^2. \quad (\text{A } 1)$$

757 Since $\mathbf{v}^n = \exp(A^{ref} n \Delta t) \mathbf{v}^0$ for all n , we have also $\mathbf{v}^{n+1} - \mathbf{v}^n = \exp(A^{ref} \Delta t) \mathbf{v}^n$. So (A 1) is
758 equivalent to

$$759 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \sum_{i=0}^{N-1} \left\| \left(\frac{\exp(A^{ref} \Delta t) - I}{\Delta t} - A \right) \mathbf{v}^n \right\|^2 = \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \left\| \left(\frac{\exp(A^{ref} \Delta t) - I}{\Delta t} - A \right) \mathbb{X} \right\|_F^2$$

760 with $\mathbb{X} = [\mathbf{v}^0, \mathbf{v}^1, \dots, \mathbf{v}^{N-1}] \in \mathcal{M}_{KN}(\mathbb{R})$. The first-order optimality conditions are

$$761 \quad A \mathbb{X} \mathbb{X}^T = \left(\frac{\exp(A^{ref} \Delta t) - I}{\Delta t} \right) \mathbb{X} \mathbb{X}^T.$$

762 As soon as \mathbb{X} is a full-rank matrix (meaning that $N \geq K$ and we reasonably have K linearly
763 independent measurements of \mathbf{v}^n), the matrix $\mathbb{X} \mathbb{X}^T$ is invertible and we get the estimate

$$764 \quad A = \frac{\exp(A^{ref} \Delta t) - I}{\Delta t}. \quad (\text{A } 2)$$

765 Let us denote by λ_k^{ref} (resp. λ_k) the (complex) eigenvalues of A^{ref} (resp. A). We have

766 $\lambda_k = \frac{e^{\lambda_k^{ref} \Delta t} - 1}{\Delta t}$. Suppose now that we use a small time step Δt . From a Taylor expansion,
767 we observe that

$$768 \quad \lambda_k = \lambda_k^{ref} + \frac{\Delta t}{2} (\lambda_k^{ref})^2 + o(\Delta t).$$

769 We would like to study what is the effect of the first-order error term $\frac{\Delta t}{2} (\lambda_k^{ref})^2$ on the
770 stability of the reconstructed dynamical system $\dot{\mathbf{v}} = A \mathbf{v}$. Suppose that the complex number
771 λ_k^{ref} has real and imaginary parts a and b respectively. Then

$$772 \quad \lambda_k = \left(a + \frac{\Delta t}{2} (a^2 - b^2) \right) + ib(1 + a\Delta t) + o(\Delta t).$$

773 If $a = \text{Re}(\lambda_k^{ref}) \leq 0$, what are the conditions to keep $\text{Re}(\lambda_k) \leq 0$? We consider two cases:

774 • If $a = 0$ (with $b \neq 0$), λ_k^{ref} is pure imaginary, meaning that the k -th field is a center for
775 the reference dynamical system. In this case $\lambda_k = -\frac{\Delta t}{2} b^2 + o(\Delta t) < 0$ for a small enough Δt .

776 • Consider now the case $a \neq 0$. There are two sub-cases. If $a^2 \leq b^2$, then $\text{Re}(\lambda_k) \leq 0$ for a
777 small enough Δt . If $a^2 > b^2$, the condition $\text{Re}(\lambda_k) \leq 0$ gives

$$778 \quad \Delta t + o(\Delta t) = -\frac{2a}{a^2 - b^2}.$$

779 So there is again a time step $\Delta t^* > 0$ for which, for any $\Delta t < \Delta t^*$ we have $\text{Re}(\lambda_k) \leq 0$.

780 As a conclusion, starting from a stable linear dynamical system (in the sense that
781 $\text{Re}(\lambda_k^{ref}) \leq 0$ for all k), using a small enough time step Δt and the forward Euler time
782 discretization, the identification method leads to an estimated dynamical system which is
783 also stable.

784 Let us underline that this could not be the case using another time discretization as e.g. for

785 the backward Euler time discretization and the associated least square problem

$$786 \quad \min_{A \in \mathcal{M}_K(\mathbb{R})} \frac{1}{2} \sum_{i=0}^{N-1} \left\| \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} - A \mathbf{v}^{n+1} \right\|^2. \quad (\text{A } 3)$$

787 Using identical developments, we would get in this case $A = \frac{I - \exp(-A^{ref} \Delta t)}{\Delta t}$ and

$$788 \quad \lambda_k = \left(a - \frac{\Delta t}{2} (a^2 - b^2) \right) + ib(1 - a\Delta t) + o(\Delta t).$$

789 We observe that for a center with a pure imaginary eigenvalue $\lambda_k^{ref} = ib$, $b \neq 0$, one gets
 790 $\lambda_k = \frac{\Delta t}{2} b^2 + o(\Delta t)$ therefore $\lambda_k > 0$ for a small enough Δt . This is a counter-intuitive result:
 791 for numerical simulations, it is known that the backward Euler scheme provide more stability
 792 than the forward one. For system identification with time discretization of the residual term,
 793 it is safer to use the forward Euler scheme for stability of the estimated dynamical model.

794 **Appendix B. Kinetic energy dissipation**

Another quantity of interest is the capsule kinetic energy $\|\{v\}\|^2$. Since the capsules are expected to reach a steady state after a transient stage in the Stokes pipe flow, the kinetic energy should also reach a constant value. From the differential equations, semi-orthogonality of Q and symmetry property of the scalar product, we successively have

$$\begin{aligned} \frac{d}{dt} \left(\frac{1}{2} \|\{v\}\|^2 \right) &= \frac{d}{dt} \left(\frac{1}{2} \langle Q\boldsymbol{\beta}, Q\boldsymbol{\beta} \rangle \right) \\ &= \frac{d}{dt} \left(\frac{1}{2} \|\boldsymbol{\beta}\|^2 \right) \\ &= \langle \boldsymbol{\beta}, \dot{\boldsymbol{\beta}} \rangle \\ &= \langle \boldsymbol{\beta}, A_\mu \boldsymbol{\beta} \rangle \\ &= \frac{1}{2} \langle \boldsymbol{\beta}, A_\mu \boldsymbol{\beta} \rangle + \frac{1}{2} \langle \boldsymbol{\beta}, A_\mu^T \boldsymbol{\beta} \rangle \\ &= \langle \boldsymbol{\beta}, \frac{A_\mu + A_\mu^T}{2} \boldsymbol{\beta} \rangle. \end{aligned}$$

795 So stability properties on the kinetic energy are related to the spectral nature of the
 796 (symmetric) matrix $A_\mu^S = \frac{A_\mu + A_\mu^T}{2}$. Dissipation property is linked to the non-positiveness
 797 of the (real) eigenvalues of A_μ^S .

798 **Appendix C. Practical computation of the pseudo-inverse matrix**

799 The Moore-Penrose pseudo-inverse \mathbb{X}^\dagger of a matrix \mathbb{X} of size $d \times K$, $d \geq K$, with $\text{rank}(\mathbb{X}) = K$
 800 is defined by

$$801 \quad \mathbb{X}^\dagger = \mathbb{X}^T (\mathbb{X}\mathbb{X}^T)^{-1}. \quad (\text{C } 1)$$

802 For an ill-conditioned matrix \mathbb{X} , the direct computation of \mathbb{X}^\dagger by formula (C 1) is unsuitable
 803 because the condition number of $\mathbb{X}\mathbb{X}^T$ is the square of that of \mathbb{X} . A more robust procedure
 804 can be derived by help of the QR factorization. There exists a semi-orthogonal matrix \hat{Q}
 805 of size $d \times K$ and an upper triangular square matrix R of size $K \times K$ such that $\mathbb{X}^T = \hat{Q}R$.

806 Moreover, R is invertible because \mathbb{X} is assumed to be a full-rank matrix. Since \mathbb{X}^\dagger is the
807 solution of the matrix system

$$808 \quad \mathbb{X}^\dagger (\mathbb{X}\mathbb{X}^T) = \mathbb{X}^T,$$

809 we get

$$810 \quad \mathbb{X}^\dagger R^T \hat{Q}^T \hat{Q} R = \hat{Q} R.$$

811 By multiplying by R^{-1} to the right, since $\hat{Q}^T \hat{Q} = I_K$ we get

$$812 \quad \mathbb{X}^\dagger = \hat{Q} (R^T)^{-1}.$$

REFERENCES

- 813 ABUHAMDAN, R. M., AL-ANATI, B. H., AL THAHER, Y., SHRAIDEH, Z. A., ALKAWAREEK, M. Y. &
814 ABULATEEF, S. R. 2021 Aqueous core microcapsules as potential long-acting release systems
815 for hydrophilic drugs. *International Journal of Pharmaceutics* **606**, 120926.
- 816 ASCHER, U. M. & PETZOLD, L. R. 1998 Computer Methods for Ordinary Differential Equations and
817 Differential-Algebraic Equations, 1st edn. USA: Society for Industrial and Applied Mathematics.
- 818 ASTER, R. C., BORCHERS, B. & THURBER, C. H. 2019 Parameter Estimation and Inverse Problems, third
819 edition edn. Elsevier.
- 820 BARRAULT, M., MADAY, Y., NGUYEN, N.C. & PATERA, A.T. 2004 An 'impirical interpolation' method:
821 application to efficient reduced basis discretization of partial differential equations. *C.R.*
822 *Mathematique* **339**, 667 – 672.
- 823 BARTHÈS-BIESEL, D., WALTER, J. & SALSAC, A.-V. 2010 Computational hydrodynamics of capsules and
824 biological cells, chap. Flow-induced deformation of artificial capsules, pp. 35–70. Taylor & Francis.
- 825 BERKOOZ, G., HOLMES, PH. & LUMLEY, J. 1993 The proper orthogonal decomposition in the analysis of
826 turbulent flows. *Ann. Rev. Fluid Mech.* **25**, 539 – 575.
- 827 BOUBEHZIZ, T., QUESADA-GRANJA, C., DUPONT, C., VILLON, P., VUYST, F. DE & SALSAC, A.-V. 2021 A data-
828 driven space-time-parameter reduced-order model with manifold learning for coupled problems:
829 Application to deformable capsules flowing in microchannels. *Entropy* **23** (9).
- 830 CASANOVA, F. & SANTOS, L. 2016 Encapsulation of cosmetic active ingredients for topical application – a
831 review. *Journal of Microencapsulation* **33** (1), 1–17.
- 832 DE VUYST, F., DUPONT, C. & SALSAC, A.-V. 2022 Space-time-parameter pca for data-driven modeling
833 with application to bioengineering. In Advances in Principal Component Analysis (ed. Prof. Fausto
834 Pedro García Márquez), chap. 13. Rijeka: IntechOpen.
- 835 DUBUISSON, M. . & JAIN, A. K. 1994 A modified hausdorff distance for object matching. In Proceedings of
836 12th International Conference on Pattern Recognition, , vol. 1, pp. 566–568 vol.1.
- 837 DUPONT, C., DELAHAYE, F., BARTHÈS-BIESEL, D. & SALSAC, A.-V. 2016 Stable equilibrium configurations
838 of an oblate capsule in simple shear flow. *J. Fluid Mech.* **791**, 738–757.
- 839 DUPONT, C., SALSAC, A.-V. & BARTHÈS-BIESEL, D. 2013 Off–plane motion of a prolate capsule in shear flow.
840 *J. Fluid Mech.* **721**, 180 – 198.
- 841 DUPONT, C., SALSAC, A.-V., BARTHÈS-BIESEL, D., VIDRASCU, M. & TALLEC, P. LE 2015 Influence of bending
842 resistance on the dynamics of a spherical capsule in shear flow. *Physics of Fluids* **27** (5), 051902.
- 843 FOESSEL, E., WALTER, J., SALSAC, A.-V. & BARTHÈS-BIESEL, D. 2011 Influence of internal viscosity on the
844 large deformation and buckling of a spherical capsule in a simple shear flow. *J. Fluid Mech.* **672**,
845 477 – 486.
- 846 GHIMAN, R., POP, R., RUGINA, D. & FOCSAN, M. 2022 Recent progress in preparation of microcapsules with
847 tailored structures for bio-medical applications. *Journal of Molecular Structure* **1248**, 131366.
- 848 HU, X.-Q., SALSAC, A.-V. & BARTHÈS-BIESEL, D. 2012 Flow of a spherical capsule in a pore with circular
849 or square cross–section. *J. Fluid Mech.* **705**, 176 – 194.
- 850 KUTZ, J., BRUNTON, S., BRUNTON, B. & PROCTOR, J. 2016 Dynamic Mode Decomposition: Data-Driven
851 Modeling of Complex Systems. SIAM.
- 852 LAC, E. & BARTHÈS-BIESEL, D. 2005 Deformation of a capsule in simple shear flow: effect of membrane
853 prestress. *Phys. Fluids* **17**, 0721051 – 0721058.
- 854 LEFEBVRE, Y. & BARTHÈS-BIESEL, D. 2007 Motion of a capsule in a cylindrical tube: effect of membrane
855 pre–stress. *J. Fluid Mech.* **589**, 157 – 181.

- 856 LI, X. & SARKAR, K. 2008 Front tracking simulation of deformation and buckling instability of a liquid
857 capsule enclosed by an elastic membrane. *J. Comput. Phys.* **227**, 4998 – 5018.
- 858 LIN, T., WANG, Z., WANG, W. & SUI, Y. 2021 A neural network-based algorithm for high-throughput
859 characterisation of viscoelastic properties of flowing microcapsules. *Soft Matter* **17**, 4027–4039.
- 860 LUMLEY, J. L. 1967 The structure of inhomogeneous turbulent flows. *Atmospheric turbulence and radio*
861 *wave propagation* pp. 166–178.
- 862 MA, G. & SU, Z.-G. 2013 Microspheres and Microcapsules in Biotechnology: Design, Preparation and
863 Applications. Pan Stanford Publishing.
- 864 MATSUNAGA, D., IMAI, Y., OMORI, T., ISHIKAWA, T. & YAMAGUCHI, T. 2014 A full gpu implementation
865 of a numerical method for simulating capsule suspensions. *Journal of Biomechanical Science and*
866 *Engineering* **9** (3), 1–16.
- 867 MIYAZAWA, K., YAJIMA, I., KANEDA, I. & YANAKI, T. 2000 Preparation of a new soft capsule for cosmetics.
868 *J. Cosmet. Sci.* **51**, 239 – 252.
- 869 POZRIKIDIS, C. 1992 Boundary Integral and Singularity Methods for Linearized Viscous Flow. Cambridge
870 University Press.
- 871 QUARTERONI, A., MANZONI, A. & NEGRI, F. 2016 Reduced basis methods for partial differential equations -
872 An introduction. Springer International Publishing.
- 873 QUESADA, C., VILLON, P. & SALSAC, A.-V. 2021 Real-time prediction of the deformation of microcapsules
874 using proper orthogonal decomposition. *J. Fluids Struct.* **101**, 103193.
- 875 RAMANUJAN, S. & POZRIKIDIS, C. 1998 Deformation of liquid capsules enclosed by elastic membranes in
876 simple shear flow: Large deformations and the effect of capsule viscosity. *J. Fluid Mech.* **361**, 117 –
877 143.
- 878 SCHMID, P. J. 2010 Dynamic mode decomposition of numerical and experimental data. *J. Fluid Mech.* **656**,
879 5–28.
- 880 SHAWE-TAYLOR, J. & CRISTIANINI, N. 2004 Kernel methods for pattern analysis. Cambridge University
881 Press.
- 882 SIROVICH, L. 1987 Turbulence and the dynamics of coherent structures, parts i, ii and iii. *Quart. Appl. Math.*
883 pp. 561–590.
- 884 TRAN, S. B. Q., LE, Q. T., LEONG, F. Y. & LE, D. V. 2020 Modeling deformable capsules in viscous flow
885 using immersed boundary method. *Phys. Fluids* **32** (9), 093602.
- 886 TRISCHLER, A.P. & D'EULEUTERIO, G.M.T. 2016 Synthesis of recurrent neural networks for dynamical
887 system simulation. *Neural Netw.* **80**, 67 – 78.
- 888 TU, J. H., ROWLEY, C. W., LUCHTENBURG, D. M., BRUNTON, S. L. & KUTZ, J. NATHAN 2014 On dynamic
889 mode decomposition: Theory and applications. *J. Comp. Dyn.* **1** (2), 391–421.
- 890 WALTER, J., SALSAC, A.-V. & BARTHÈS-BIESEL, D. 2011 Ellipsoidal capsules in simple shear flow: prolate
891 versus oblate initial shapes. *J. Fluid Mech.* **676**, 318 – 347.
- 892 WALTER, J., SALSAC, A.-V., BARTHÈS-BIESEL, D. & LE TALLEC, P. 2010 Coupling of finite element and
893 boundary integral methods for a capsule in a Stokes flow. *Int. J. Num. Meth. Engng* **83**, 829 – 850.
- 894 WILLIAMS, M.O., KEVREKIDIS, I.G. & ROWLEY, C.W. 2015 A driven-approximation of the koopman operator:
895 Extending dynamic mode decomposition. *J. Nonlinear Sci.* **25**, 1307 – 1346.
- 896 YE, T., SHI, H., PENG, L. & LI, Y. 2017 Numerical studies of a red blood cell in rectangular microchannels.
897 *J. Appl. Phys.* **122** (8), 084701.
- 898 YUN, P., DEVAHASTIN, S. & CHIEWCHAN, N. 2021 Microstructures of encapsulates and their relations with
899 encapsulation efficiency and controlled release of bioactive constituents: A review. *Comprehensive*
900 *Reviews in Food Science and Food Safety* **20** (2), 1768–1799.
- 901 ZHAO, H., ISFAHANI, A. H.G., OLSON, L. N. & FREUND, J. B. 2010 A spectral boundary integral method for
902 flowing blood cells. *Journal of Computational Physics* **229** (10), 3726–3744.