

RESEARCH STATEMENT

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My research focuses on analytical and computational modeling of problems arising in the dynamics of fluids and their interactions with a solid or a liquid phase. One of the most challenging issues one faces in modeling such problems is the coupling of the physics at the smallest scales with observable behaviors at the larger scales. My research addresses the theoretical, stochastic and numerical aspects of such systems and the inherent simplifications often being made in their description. Since arriving at Utah, I have tackled many different problems motivated by intriguing fluid behaviors, often stemming from biological applications and I will describe them in the subsequent paragraphs. Most of my work is driven by collaboration and discussions with colleagues at Utah and elsewhere, graduate students, and undergraduate students. The result that is the most significant for its impact on the field and the future directions of my research is the rigorous derivation of a fluctuating hydrodynamics model for complex fluids. Complex fluids are omnipresent in our everyday life, as they encompass material from polymer melts, to mucus, blood, cake batter, and silly putty, with applications in engineering (mining, synthetic liquid), bioengineering (targeted drug delivery), biology (cell development, bacteria motion), and medicine (cystic fibrosis, sickle cell disease). The fluctuating hydrodynamics model for complex fluid, which I discuss in details below, is the first of its kind to model both the solvent and polymer fluctuations in a thermal bath in the form of stochastic stresses.

1 Complex fluids [27, 28, 25, 22, 26]

My interest in complex fluids goes back to discussions with Peter Mucha and Greg Forest towards the end of my Ph.D thesis, which led to a paper [26] proposing a protocol to determine the length of a depletion layer surrounding a sphere in a complex fluid. This paper was my first step towards a rigorous mathematical study of current experimental and modeling aspects of the motion of passive particles in complex fluids. Ultimately, in 2013, it led to a collaboration with Scott McKinley (Tulane) to develop models of complex fluids and passive particles that properly encapsulate thermal fluctuations. This project is supported by NSF-DMS 1413378, and it has resulted in publications [27, 28, 22, 25].

Complex fluids are liquids that contain suspended solid flexible microstructures ranging from a couple of nanometers to tens of microns in a viscous background fluid. They appear homogeneous at a scale of microns to centimeters, and they can behave as a solid or a fluid depending on the applied stress/strain [62, 46, 37, 72]. As is standard practice, we refer to the background viscous fluid as the solvent and to the suspended microstructures as the polymers. Describing the mechanical responses of a complex fluid to forcing is the aim of rheology. In the subfield of passive microrheology, the thermal fluctuations of spherical passive fluid tracers are recorded, and the mean square displacement (MSD) is used to infer the storage (elastic) and loss (viscous) moduli as a function of frequency, $G'(\omega)$ and $G''(\omega)$ respectively, characterizing the bulk fluid properties [44, 60]. There are two standard approaches to modeling the motion of a passive particle in a complex fluid as a generalization of traditional work for a viscous fluid. In the first one, pioneered by Langevin, Ornstein and Uhlenbeck [39, 57], one writes down an equation of motion (force balance) on the spherical particle. The fluid equations are never solved, instead the drag coefficient of a sphere in an unbounded fluid and the fluctuation-dissipation theorem are used to obtain the deterministic coefficient and the covariance structure. Starting from the seminal work of Mason & Weitz [45], which is justified by earlier works from Kubo [34] and Zwanzig [74], there have been attempts

to extend the Langevin's approach to complex fluids, see for example [44, 43, 32, 73, 40, 41, 42, 5]. However, these models only consider the polymer contribution focusing mostly on the restrictive class of Maxwell fluids. Our contribution to this field is to include the solvent contribution and to fill in the theoretical gap in the derivation of the equations. In the second approach, proposed by Landau-Lifshitz [52] and later used by Atzberger *et al.* [4, 33] and Donev *et al.* [10, 9], the fluid equations are solved with added fluctuations in the form of stochastic stresses. The particle is then passively advected. Our work is the first one to generalize this framework to complex fluids. The deep dependencies between both frameworks were highlighted by the results of Sutherland [64], Einstein [12, 13] and Smulochowski [70] for viscous fluids. It is therefore not surprising that similar dependencies exist for complex fluids, however they remain poorly understood and my overall long term goal is to explain them as rigorously as possible.

In the following paragraphs, I describe in detail our model that extends the Landau-Lifshitz-Navier-Stokes framework [52] to linear viscoelastic fluids combining both solvent and polymer contributions described in [27]. Consider the incompressible Navier-Stokes equation for a fluid velocity field \mathbf{u} without external forces

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = \nabla \cdot \boldsymbol{\Sigma}, \quad \text{and} \quad \nabla \cdot \mathbf{u} = 0, \quad (1)$$

where ρ is the fluid density. $\boldsymbol{\Sigma}$ is the total stress tensor comprised of two components: a deterministic viscoelastic stress $\boldsymbol{\Sigma}_{\text{det}}$ and a stochastic stress $\boldsymbol{\Sigma}_{\text{stoch}}$. The deterministic stress tensor can be decomposed into a solvent contribution $\boldsymbol{\Sigma}_{\text{det},s}$ and a polymeric contribution $\boldsymbol{\Sigma}_{\text{det},p}$ [38]. The solvent stress is Newtonian: $\boldsymbol{\Sigma}_{\text{det},s} = -p\mathbf{I} + 2\eta_s \mathbf{E}$, where p is the pressure, \mathbf{I} is the identity matrix, and $\mathbf{E} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ is the rate-of-strain tensor. As in [60, 73, 16, 38], we consider the small strain limit resulting in a linear viscoelastic model, known as the Lodge equation. It has the form

$$\boldsymbol{\Sigma}_{\text{det},p} = G_{\text{avg}} \mathbf{I} + 2 \int_{-\infty}^t G_r(t-t') \mathbf{E}(t') dt', \quad (2)$$

where G_{avg} is the mean stress and $G_r(t)$ is the relaxation modulus, such that $G_r(t) = 0$ for $t < 0$ (causal). There are random fluctuations in the stress tensor due to thermal energy. As with the deterministic stress tensor, we separate $\boldsymbol{\Sigma}_{\text{stoch}}$ into two terms: $\boldsymbol{\Sigma}_{\text{stoch},s}$ and $\boldsymbol{\Sigma}_{\text{stoch},p}$. Following Landau-Lifshitz, the solvent fluctuation has the form $\boldsymbol{\Sigma}_{\text{stoch},s} = \sqrt{2k_B T \eta_s} \dot{\mathbf{W}}$, where $\dot{\mathbf{W}}$ is a space-time white noise tensor with

$$\mathbb{E} [\dot{W}_{ij}(\mathbf{x}, t) \dot{W}_{mn}(\mathbf{y}, s)] = (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) \delta(\mathbf{x} - \mathbf{y}) \delta(t - s). \quad (3)$$

The polymer fluctuation has the form $\boldsymbol{\Sigma}_{\text{stoch},p} = \sqrt{k_B T \eta_p / \tau_{\text{avg}}} \mathbf{F}$ where \mathbf{F} is a stationary, mean zero Gaussian process that is white in space, but not in time. In accordance with the fluctuation-dissipation theorem, the memory structure of the thermal fluctuations matches that of the deterministic part:

$$\mathbb{E} [F_{ij}(\mathbf{x}, t) F_{mn}(\mathbf{y}, s)] = (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) \delta(\mathbf{x} - \mathbf{y}) K(t - s) \quad (4)$$

where K is the dimensionless memory kernel defined as $G_r(t) = \frac{\eta_p}{\|K\|_1} K(t) 1_{t \geq 0}$, where η_p is the polymer viscosity. To simplify Eq. (5), we perform a dimensional analysis by choosing the dissipative time scale $L^2 \rho / \eta_s$ as the characteristic time, the length L as the characteristic length (periodic domain of length $2\pi L$) and the velocity $\sqrt{k_B T / \rho L^3}$ as the characteristics velocity. We find two dimensionless groups: the Reynolds number and $\beta = \eta_p \rho L^2 / (\|K\|_1 \eta_s^2)$. Assuming small Reynolds number, we have

$$\partial_t \mathbf{u} = -\nabla p + \Delta \mathbf{u} + \beta \int_{-\infty}^t K(t-s) \Delta \mathbf{u}(s) ds + \sqrt{2} \nabla \cdot \dot{\mathbf{W}} + \sqrt{\beta} \nabla \cdot \mathbf{F} \quad \text{and} \quad \nabla \cdot \mathbf{u} = 0. \quad (5)$$

If the solvent is water, $L = 10 \mu\text{m}$ and $\eta_p / \|K\|_1 = 10^{-4} \text{mg/ms}^{-2}$, then $\beta \approx 10$. Upon transforming Eq. (5) into Fourier space, and projecting into the space of incompressible solutions, it can be shown that

the projected components of each Fourier modes satisfy a Generalized Langevin Equation (GLE). The most important aspect of the derived fluctuating hydrodynamic model is that it satisfies equipartition of energy, i.e. that each Fourier mode contributes equally to the total energy. The proof of this non-trivial fact relies on the statement of equipartition of energy for a GLE with a generalized Rouse kernel, which I established in [22] using residue calculus and which is a stronger result than that of Kubo [34].

As a first approximation, a particle that is passively advected by the fluctuating fluid model in Eq. (5) can be modeled as a local average of the stochastic velocity field. The resulting particle advection equation is numerically solved with a semi-implicit Euler method where the time integral of the projected component of each fluid mode is realized exactly using the covariance of the underlying process. In [27], we established convergence of the resulting position process and of the numerical method. In this first model, the particle does not influence the fluid, even locally. This is obviously an oversimplification, as no boundary condition on the surface of the sphere has been imposed. My current and immediate goal is therefore to include the back-coupling of the particle to the fluid in a manner similar to that of Donev *et al.* [10] for viscous and compressible flows. This step will allow for the simulation of multiple particles interacting through the complex fluid. The main anticipated difficulty is that the coupling will give rise to non-Gaussian processes, and hence our numerical method will have to be adjusted by using an alternate Markovian form for the resulting underlying GLEs as described in [49, 74, 18, 47].

As the previous paragraphs suggest the fundamental component in understanding and solving the fluctuating hydrodynamic model in Eq. (5) is GLEs, which is a strong indication of the deep connection between a Langevin particle based approach and a Landau-Lisfhtz fluid based approach. The stochastic process $Y(t)$ solving a GLE is Gaussian, non-Markovian and stationary, while its integral process, formally defined as $Z(t) = \int_0^t Y(s)ds$ is a Gaussian, non-Markovian, non-stationary process. Using a derived expression for the covariance of $Y(t)$, it is possible to find an integral expression for the covariance of $Z(t)$, which can be numerically evaluated. Since the process is Gaussian, this results in a new covariance based method for realizing $Z(t)$, which is described in [22, 25]. It is also the basis for the novel, spectral and statistically accurate method I developed for the realization of paths in a fluctuating hydrodynamic complex fluid discussed in [27] and illustrated in Fig. 1(a). As an aside, the covariance based method for a GLE was applied by Ryan Durr and D. Michael Senter as part of an REU project to estimate the mean first passage time in a complex fluid described by the generalized Rouse kernel and to establish quadratic growth of the mean first passage time with the layer's width presented in [25].

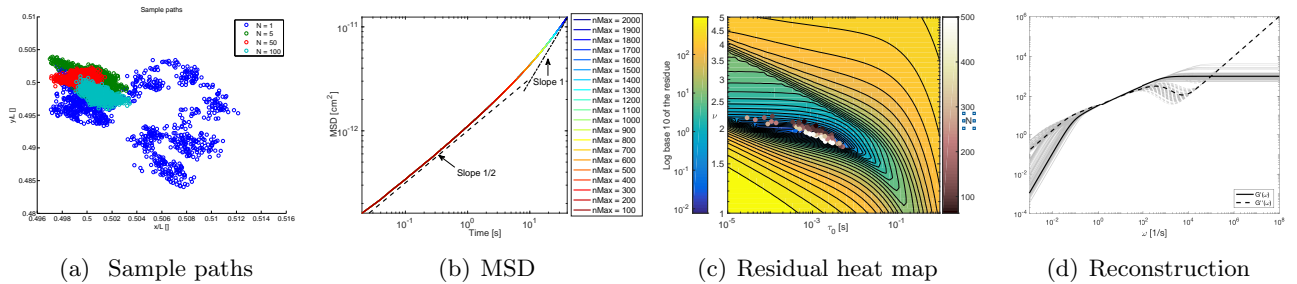


Fig. 1: Passive microrheology: Reconstruction of bulk fluid properties from MSD data in complex fluids.

In our most recent paper [28], we frame the inference problem of passive microrheology as an inverse problem and are the first to quantify in a systematic way the uncertainties in extracting the bulk fluid properties $G'(\omega)$, $G''(\omega)$ in the frequency domain from MSD in the time domain. Assuming that the solvent viscosity η_s is known and that the memory kernel $K(t)$ is a generalized Rouse kernel, then $G_r(t)$ is uniquely determined by η_p the polymer viscosity, τ_0 the smallest relaxation time in $K(t)$, N the number of terms in $K(t)$ and ν the subdiffusive exponent. The subdiffusive exponent is the slope (less than one)

of the MSD on a log-log plot before the transition to pure diffusion (slope one) and it is illustrated in Fig. 1(b) ($\nu = 2$, slope $1/2$), where n_{Max} and the associated color is the length of the path. Performing a nonlinear weighted least square optimization on simulated data, we demonstrate that the parameters η_p, τ_0, N, ν are practicably unidentifiable. This means that if one parameter is overestimated, then another one can be underestimated to give a minimal residue. This phenomena is shown by the residual heat map in Fig. 1(c), where the blue to yellow color bar represents the minimal residue in N, η_p for each τ_0, ν and each cordovan colored N dot is the result of one optimization. While the residual map is the central result of [28], from an experimental point of view, it is the storage and loss moduli that are important. Again, assuming a generalized Rouse kernel, $G'(\omega), G''(\omega)$ can be analytically expressed in terms of $G_r(t)$ [38]. Therefore, in Fig. 1(d), we plot $G'(\omega)$ and $G''(\omega)$ for each cordovan dot in Fig. 1(c). In [28], we also establish an auxiliary balance condition showing that $\mathbb{E}[F(t)V(0)] \neq 0$, extending a previous calculation that I had done for the generalized Rouse kernel and filling a theoretical gap in the standard theory of the inverse problem of relating MSD to bulk fluid properties [45, 44, 60].

As the model evolves, there are many questions that I wish to address in this field. They range from purely theoretical (particles cross-correlation, particle's mobility) to application to experimental data (mucus) and to extension to melts and to spatially heterogeneous and anisotropic complex fluids.

The most exciting complex fluids problem I wish to address in the near future stems from some preliminary discussions with Aaron Fogelson (Utah) and Thomas Fai (Harvard) about the potential applications of the Landau-Lifshitz-Navier Stokes framework for the numerical simulations of red blood cells, white blood cells and platelets in blood flow. The idea is to use previous work by Fogelson *et al.* [7, 17] to coarse grain the red and white blood cells suspensions to a complex fluctuating fluid extracting the relevant covariance structure of the fluctuations from numerical simulations and to then passively advect the non-spherical platelets.

2 Suspensions [30, 29, 6, 24, 61, 50, 23]

In the above discussion on complex fluids, constitutive equations for the contribution of the suspended microstructure to the background viscous fluid were taken from the literature, e.g. [38]. This approach is not always possible and new models of complex fluids can be obtained from first principles. Starting from my postdoctoral work with Mike Shelley [30, 29] on the stability of active suspensions, I have been interested in suspensions and their resulting coarse-grained models. This line of research has resulted in four different applications: dynamics near a boundary (publication [61]), microtubule gliding assays (publications [6, 24]), separation of binary species (new) and Arctic melt ponds (publications [50, 23]).

2.1 Dynamics near a boundary

In recent years, much has been learned about models and properties of active suspensions. For example, it has been experimentally demonstrated [31, 8, 58] that geometry and boundary conditions drive active fluids. Further, numerical and theoretical works [21, 11, 59, 48] suggest that hydrodynamic interactions between the wall and the active structures dominates the motion of a single swimmer near a wall.

In work with graduate student Kyle R. Steffen (Utah, advisors Ken Golden and Yekaterina Ephsteyn) [61], we generalize slender body theory to objects near a stationary wall. Slender body theory is a common modeling approach for describing swimming organisms, where the motile force is due to an imposed shear stress at the particle surface and the dynamics of the slender particle is approximated by relating its velocity to the force along its center-

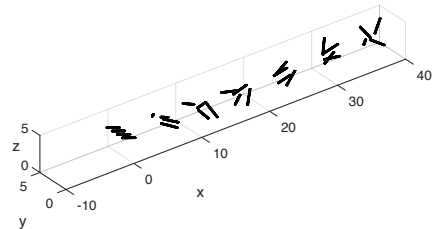


Fig. 2: Slender bodies sedimenting near a stationary wall.

line [53, 54]. In free space, only the local drag model is considered, but because interactions between a suspended particle and a fixed wall are inherently nonlocal, higher order, nonlocal terms must be kept in the asymptotic expansion. Motivated by the works of Tornberg *et al.* [68, 67] on sedimenting fiber suspensions and of Götz [19] on slender body theory in free space, we develop a nonlocal slender body theory above a stationary planar wall using asymptotic analysis of the nonlocal interaction terms up to order $O(a)$ (a radius). Interestingly, the wall Stokeslet and wall source dipole strengths along the centerline satisfy the same relationship as in free space [19]. The resulting dynamics of M particles requires solving a system of coupled integral equations for the force density, which is discretized using a Legendre polynomial expansion as in [67]. Our numerical experiments illustrated in Fig. 2 show good agreement with the gliding and bouncing of particles near a wall observed in [48] and the sedimenting of particles under gravity in free space observed in [20].

2.2 Microtubule gliding assays

In work with Tamar Shinar (UC Riverside, CS) and her graduate student Steve Cook [6, 24], we undertook the task of developing a continuum model describing a mixture of microtubules and molecular motors in an in-vitro microfluidic device known as a gliding assay from first principles. When the molecular motors are held fixed to a bottom plate, the motion of the microtubules has been shown experimentally to lead to the emergence of organized structures like coherent swarms, density waves or vortex lattices [55, 63]. In contrast to other modeling approaches, we use continuum theories to connect the small scales stepping motion of the molecular motors to the large scale flow field and present a first micro-macro fluid-mediated model of gliding assays with qualitative features of the experiments.

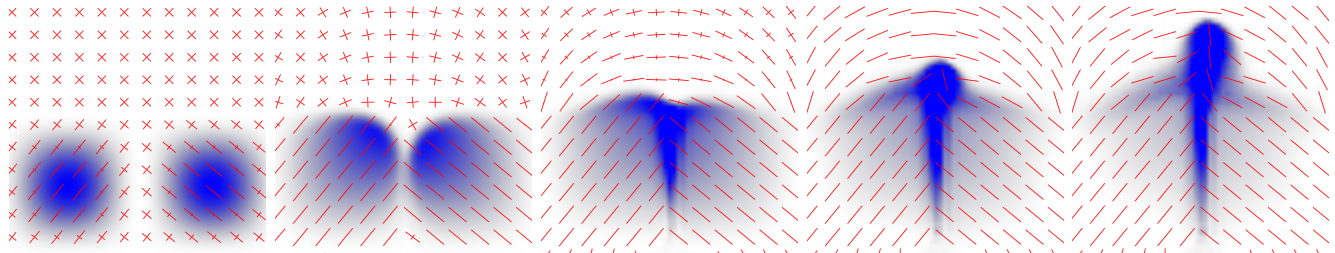


Fig. 3: Nearly perpendicular concentrated microtubule clumps colliding and merging.

There are four main components to the continuum model: a microtubule conservation equation, an equation for bound motors, an equation for free motors and fluid equations. The filament conservation equation allows for the consideration of concentrated suspensions by the inclusion of steric and hydrodynamic terms treated in the same way as for suspensions of active particles [15]. The fluid equations are modeled using Stokes equations with extra stresses arising from inextensibility and steric interactions and forces due to the activity of the motors spread directly to the fluid. As a result, the microtubules are passively advected by the fluid. The conversion between bound and free motors is achieved locally in a caption region. There are two possible ways to reduce the complexity of the model. In our first paper [24], we neglect sterics interactions and average all equations over the height of the channel adopting a Hele-Shaw approach and a dimensional reduction analysis. On the other hand, in our follow-up paper [6], we keep both steric and hydrodynamics contributions and assume that the microtubules are constrained to move in a plane located slightly above the bottom wall. In either case, the resulting system of PDEs is high dimensional and must be solved on GPUs. As for the numerical method, we use a combination of finite difference methods (Crank-Nicolson, Adams-Bashforth 2, and flux limiter) for the microtubules and motors and spectral methods for the fluid. Optimal management of memory can be achieved by

realizing that motors can only attach in a local grid around any spatial point. We use our simulations to test various experimental set-up like break-up, collision, or traveling of clumps. One such example from our second paper is given in Fig. 3, which shows two highly concentrated and locally aligned clumps of filaments colliding. The filament concentration is shaded in blue, while the local nematic alignment is represented by the red crosses. We conclude that pure hydrodynamics coupling in a dilute suspension of microtubules is enough to reproduce swirls and high-density front motion, while steric interactions are necessary in a concentrated suspension to reproduce the formation, merging and splitting of clumps of filaments.

2.3 Separation of binary species

In a new project with graduate student Becky Terry (Utah), whose Ph.D thesis (advisor Fred Adler) focuses on population dynamics in fluctuating environment, we are interested in developing a continuum model for two binary species that can be separated by applications of an external field and in studying the stability and bifurcation structure of the resulting dynamical system. The underlying question is to understand how density fluctuations affect the development of a population. This question is motivated by discussion with Henry Fu (Utah, ME) and by recent work on magnetically separated microbots [3].

2.4 Melt ponds

During the Arctic melt season, the sea ice surface transforms from vast expanses of snow covered ice to complex mosaics of ice and melt ponds (see Fig. 4). Despite the central role that melt ponds play in understanding the decline of the summer Arctic sea ice pack, comprehensive observations or theories of their formation, coverage, and evolution remain relatively sparse.

In work with Ken Golden's group [50, 23], I investigated the existence of universal features in melt pond evolution. To achieve this, I analyzed area-perimeter data obtained from hundreds of thousands of segmented images using Matlab image processing toolbox. The geometrical features of melt ponds and the complexity of their boundaries can be captured by the fractal dimension D , defined as $P \sim \sqrt{A}^D$, where A and P are the area and perimeter, respectively. D can be determined on a log-log plot of the $A - P$ data as twice the slope. For regular objects, the perimeter scales like \sqrt{A} , and $D = 1$. For melt ponds, I found an unexpected separation of scales, where D transitions from 1 to 2 around a critical length scale of 100 m^2 in area. This can be understood by the fact that pond complexity increases rapidly through the transition as smaller ponds coalesce to form large connected regions, and reaches a maximum for ponds larger than 100 m^2 whose boundaries resemble space filling curves with $D \approx 2$.

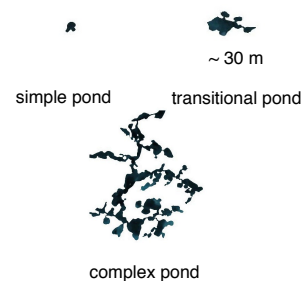


Fig. 4: Melt ponds

3 Sloshing Dynamics [66, 65]

A more recent interest of mine has been sloshing dynamics, in other words the study of the movement of a fluid inside a container. Of particular interests are the shape of the free surface between the liquid and the air and of the container, as it relates to the propensity of the liquid to spill. In current work with graduate student Chee Han Tan (Utah) co-advised with Braxton Osting, we have been considering the sloshing problem for an incompressible, inviscid, irrotational fluid in a container, including the effects of surface tension on the free surface. Surface tension, which is a measure of the tensile force at the interface resulting from the pressure differential between the air and the liquid, is believed to play a major role in controls of satellites and space probes [14], and sloshing of liquid propellants has been deemed by

NASA the main cause of multiple missions' failure, e.g. [2, 1, 56, 36]. Recent advances in computational fluid dynamics have made accurate numerical modeling of sloshing dynamics possible [51]. However, it requires extensive experimental validation and verification in microgravity environment, and is extremely expensive. Our goal is to provide some insights into these and related questions by studying the linearized problem, which has not been done previously.

The equations of sloshing dynamics are derived from the Navier-Stokes equations for an incompressible, ideal and irrotational fluid. On the solid wall of the container, no flux boundary conditions are imposed, while the kinematic condition at the moving interface is that particles on the free surface remains on it as the flow evolves. The resulting set of PDEs and boundary conditions are then linearized away from the rest state and time harmonic solutions are sought. In our first paper [66], we restrict ourselves to a constant contact angle. The dimensionless number that measures the importance of gravitational forces to surface tension forces is the Bond number, Bo . In the absence of surface tension, $Bo \rightarrow \infty$, our model reduces to the Stekelov eigenvalue problem for the velocity potential discussed in [69, 35]. However, if surface tension is not negligible, we obtain a coupled system for the velocity potential and the free surface displacement. The system is solved using a new variational formulation and the associated minimization problem for the first non-trivial sloshing eigenvalue is

$$\inf_{(\Phi, \xi) \in \mathbf{H}} D[\Phi] + S[\xi] \quad \text{subject to} \quad \langle \Phi, \xi \rangle_{L^2(\mathcal{F})} = 1, \quad (6)$$

where $\mathbf{H} = \{(\Phi, \xi) \in H^1(\mathcal{D}) \times H^1(\mathcal{F}) : \int_{\mathcal{F}} \Phi dA = \int_{\mathcal{F}} \xi dA = 0\}$, $D[\Phi] = \frac{1}{2} \int_{\mathcal{D}} |\nabla \Phi|^2 dV$ is the Dirichlet energy and $S[\xi] = \frac{1}{2} \int_{\mathcal{F}} (\xi^2 + \frac{1}{Bo} |\nabla_{\mathcal{F}} \xi|^2) dA$ is the free surface energy. In Eq. (6), Φ is the velocity potential, ξ is the free surface elevation, \mathcal{D} is the fluid domain and \mathcal{F} is the free surface.

In an REU project with Max Carlson [65], we propose a finite-element numerical method for computing the sloshing modes of the linearized coupled system, which works for arbitrary containers and is illustrated in Fig. 5. When put in a finite-element form, the coupled PDE system reduces to a generalized eigenvalue problem. The generation of the meshes and matrices is done using Hari Sundar's code (Utah, CS).

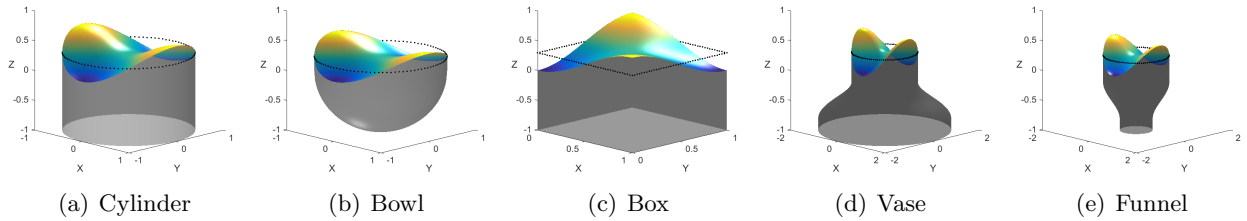


Fig. 5: Sloshing surfaces with surface tension in different containers ($Bo=10$).

In our first approach [66, 65], we made the major assumptions that the container walls were straight and that the contact angle was 90 degrees. We are currently working on a more general set of equations that couples Navier-Stokes for a viscous fluid to the dynamic of the contact line (the intersection between the three phases), which was studied on its own by Weiquing and Weinan [71]. There are many interesting optimization questions that can be addressed in a more general framework, such as finding the optimal shape of the container that minimizes sloshing (isoperimetric problem) or the shape of the container such that the first sloshing frequency is always the same, independent of the liquid's height (isochronous problem). Another question is, how to generalize the analysis to include surfactants on the surface and to describe the fundamental oscillation of a layer of foam on a free surface in a container.

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