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Artificial viscosity model to mitigate numerical artefacts at fluid interfaces with surface tension

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ABSTRACT

The numerical onset of parasitic and spurious artefacts in the vicinity of fluid interfaces with surface tension is an important and well-recognised problem with respect to the accuracy and numerical stability of interfacial flow simulations. Issues of particular interest are spurious capillary waves, which are spatially underresolved by the computational mesh yet impose very restrictive time-step requirements, as well as parasitic currents, typically the result of a numerically unbalanced curvature evaluation. We present an artificial viscosity model to mitigate numerical artefacts at surface-tension-dominated interfaces without adversely affecting the accuracy of the physical solution. The proposed methodology computes an additional interfacial shear stress term, including an interface viscosity, based on the local flow data and fluid properties that reduces the impact of numerical artefacts and dissipates underresolved small scale interface movements. Furthermore, the presented methodology can be readily applied to model surface shear viscosity, for instance to simulate the dissipative effect of surface-active substances adsorbed at the interface. The presented analysis of numerical test cases demonstrates the efficacy of the proposed methodology in diminishing the adverse impact of parasitic and spurious interfacial artefacts on the convergence and stability of the numerical solution algorithm as well as on the overall accuracy of the simulation results.

1. Introduction

The dynamics of an interface separating two immiscible fluids is governed by the behaviour of individual molecules, which typically have a size of less than one nanometer. Computational fluid dynamics (CFD), however, is based on continuum mechanics and treats fluids as continuous media. Molecular scales cannot be resolved using continuum mechanics, which leads to a variety of theoretical and numerical difficulties with respect to the representation of fluid interfaces using CFD. These difficulties manifest as parasitic (of unphysical origin) or spurious (of physical origin but numerically misrepresented) flow features in the vicinity of the interface. Numerical artefacts of particular practical interest in interfacial flow modelling that have attracted significant attention and research efforts are parasitic currents [1–7] and spurious capillary waves [1,8–13].

The numerical onset of unphysical flow currents in the vicinity of the interface, so-called *parasitic currents*, are a common occurrence in the modelling of surface-tension-dominated flows. Previous studies [3–6] have identified two distinct origins of parasitic currents: a) a discrete imbalance between pressure "jump" and surface tension and b) a numerically unbalanced evaluation of the interface curvature. The imbalance of the pressure gradient and surface tension can be eliminated by employing so-called balanced-force discretisation methods that assure a discrete balance between surface tension and pressure gradient, which has previously been proposed and successfully demonstrated by Renardy and Renardy [14] and Francois et al. [4] for sharp surface representations such as the ghost-fluid method [15,16], and by Francois et al. [4], Mencinger and Žun [5] and Denner and van Wachem [6] for methods using a continuum surface force formulation [1,17]. A numerically unbalanced evaluation of the interface curvature, which is typically associated with spatial aliasing errors resulting from the computation of the second derivative of a discrete indicator function or reconstruction [3,6], leads to an unphysical contribution to the momentum equations (via surface tension) and, consequently, causes an unphysical acceleration of the flow in the vicinity of the interface [4,7]. Using a balanced-force discretisation of the surface tension, parasitic currents are solely dependent

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on the evaluation of the interface curvature and can, for instance, be eliminated (*i.e.* reduced to machine precision) for certain cases by imposing the geometrically exact curvature [4–7]. Although previous studies [7,18] have shown that, with a careful discretisation of the interface curvature, parasitic currents can be reduced to machine precision in some cases once the interface has reached a numerical equilibrium, parasitic currents are still an issue of significant practical relevance for applications with evolving interfaces, as evident by the considerable body of literature on this subject published over the past five years alone (*e.g.* [7,19–22]).

Another important numerical artefact in interfacial flows are *spurious capillary waves*. In a numerical framework, the shortest wavelength unambiguously resolved by the computational mesh is $\lambda_{\min} = 2\Delta x$, with Δx representing the mesh spacing. Because an adequate spatial resolution of waves requires at least $6-10$ cells per wavelength [13], capillary waves with a wavelength of $\lambda_{\min} \leq \lambda \lesssim 3\lambda_{\min}$ are not part of the physical solution and can, therefore, be considered to be spurious capillary waves, meaning that these waves are a response of the discretised governing equations to a perturbation of the interface but are numerically misrepresented. Therefore, spurious capillary waves are, contrary to parasitic currents, not the result of numerical errors but the result of the limitations associated with the finite resolution of the computational mesh. The origin of spurious capillary waves can be physical perturbations of the interface, for instance due to the collision of the interface with an obstacle, as well as numerical perturbations, for instance the finite accuracy of numerical algorithms, discretisation errors or parasitic currents [13]. An adequate temporal resolution of the propagation of all spatially resolved capillary waves is essential for a stable numerical solution [1,13]. The dispersion relation of capillary waves in inviscid fluids is given as [23]

$$\omega_\sigma^2 = \frac{\sigma\, k^3}{\rho_\mathrm{a} + \rho_\mathrm{b}}\ , \tag{1}$$

from which the phase velocity follows as $c_\sigma = \omega_\sigma / k$, where ω_σ is the angular frequency of capillary waves, k is the wavenumber, σ is the surface tension coefficient and ρ is the density of the adjacent fluids a and b. Hence, the phase speed of capillary waves increases with decreasing wavelength. This anomalously dispersive behaviour of capillary waves leads to a very rigid time-step restriction for interfacial flow simulations. For the shortest spatially resolved capillary waves, Denner and van Wachem [13] devised the capillary time-step constraint as

$$\Delta t_\sigma \leq \frac{\Delta x}{\sqrt{2}\, c_\sigma + u_\Sigma}\ , \tag{2}$$

where Δx denotes the mesh spacing and u_Σ is the flow velocity tangential to the interface. Denner and van Wachem [13] demonstrated that the shortest spatially resolved capillary waves are in most cases not subject to viscous attenuation, since the computational mesh is usually too coarse for typical values of the fluid viscosities to spatially resolve the vorticity generated by the shortest numerically represented waves.

The capillary time-step constraint limits the simulation of interfacial flow applications and has been commonly attributed to the explicit numerical implementation of surface tension. As a result, it is widely postulated that an implicit implementation of surface tension would lift or at least mitigate the capillary time-step constraint [1,8–10,18]. Recent research efforts inspired by this assumption aimed at finding an implicit or semi-implicit treatment of the surface tension to lift the time-step restrictions in interfacial flows [8,9,11,12]. Hysing [8] proposed a semi-implicit formulation of surface tension based on the CSF method [1] for a two-dimensional finite element method. The semi-implicit formulation of Hysing includes an additional implicit term which represents artificial shear stresses tangential to the interface. Raessi et al. [9] translated this methodology for finite volume methods and reported that this semi-implicit formulation of surface tension allows to exceed the capillary time-step constraint by up to factor five without destabilising the solution of the presented two-dimensional test cases. Schroeder et al. [11] proposed a two-dimensional method with a semi-implicit implementation of surface tension on a Lagrangian interface mesh (*i.e.* using an explicit representation of the interface) coupled to a Eulerian mesh for the flow, presenting stable results for time-steps up to $\Delta t = 3\,\Delta t_\sigma$. In a similar fashion, Zheng et al. [12] recently proposed a fully-implicit coupling of a Lagrangian interface mesh to a MAC grid and showed that the method can yield stable results for time-steps up to $\Delta t \approx 10^3\,\Delta t_\sigma$. However, with respect to methods that rely on an implicit interface representation, such as Volume-of-Fluid methods [24] or Level-Set methods [25,26], and the CSF method of Brackbill et al. [1], Denner and van Wachem [13] demonstrated that the temporal resolution requirements associated with the propagation of capillary waves is a result of the spatiotemporal sampling of capillary waves and is independent of whether surface tension is implemented explicit or implicit. Simulating the thermocapillary migration of a spherical drop, Denner and van Wachem [13] demonstrated that without external perturbations acting at the interface (such as parasitic currents), the capillary time-step constraint can be exceeded by several orders of magnitude without destabilising the solution, presenting stable results for $\Delta t = 10^4\,\Delta t_\sigma$ using an explicit implementation of surface tension. Thus, in order to mitigate or lift the capillary time-step constraint for numerical methods that rely on an implicit interface representation, the shortest capillary waves spatially resolved by the computational mesh have to be either filtered out or damped with an appropriate method to mitigate their impact.

Issues regarding numerical artefacts are, however, not limited to interfacial flows. For instance, numerical oscillations induced by a high-order discretisation of advection terms is a longstanding issue in CFD as well as numerical heat and mass transfer, and has been the topic of extensive studies, *e.g.* [27–31]. Artificial viscosity is a well-established concept to mitigate or eliminate high-frequency oscillations in the solution and improve the stability of the numerical methodology, in particular for shock capturing and in transsonic flows, and numerical models that incorporate artificial viscosity span a wide range of explicit and implicit methods, see *e.g.* [32–37]. Cook and Cabot [35] suggested that the artificial grid-dependent viscosity should be chosen as to only damp wavenumbers close to the Nyquist wavenumber $\pi/\Delta x$, which in a numerical simulation is the wavenumber of the shortest spatially resolved waves. Discretisation schemes which introduce numerical diffusion to avoid oscillatory solutions, such as TVD schemes [27–29], are often considered to be part of the artificial viscosity models as well. In fact, TVD schemes can be readily translated into an explicit artificial viscosity term, as for instance shown by Davis [38].

In this study we propose an artificial viscosity model to mitigate numerical artefacts at fluid interfaces, expanding on the work of Raessi et al. [9]. The proposed artificial viscosity model can accommodate arbitrary interface viscosities and two methods to dynamically compute the interface viscosity based on the local flow conditions are presented. We present and discuss the results for a range of numerical experiments, which allow a comprehensive assessment of the efficacy of the methodology, highlight the acting physical mechanisms and provide best practice guidelines for future interfacial flow simulations using the proposed artificial viscosity model. Furthermore, our study demonstrates that the success of the proposed methodology with regards to mitigating the capillary time-step constraint is solely based on the dissipation of surface energy, irrespective of the type of implementation, contrary to previous suggestions [8,9].