

A Particle-Derived Nonlinear Dynamical Framework for Bubble Oscillations: Reduced-Order Modeling, Bifurcation Analysis, and Optimal Stabilization

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Abstract

Particle-based fluid simulation has emerged as a powerful computational framework for modeling complex multiphase flows involving large deformations, moving interfaces, and nonlinear fluid interactions that challenge conventional mesh-based approaches. In this work, a nonlinear dynamical systems framework is developed for particle-resolved bubble oscillations by constructing a reduced-order model that preserves the dominant physical mechanisms governing bubble interface evolution. The formulation represents the bubble dynamics through coupled radial and shape deformation modes derived from particle-based fluid behavior, incorporating inertial effects, viscous dissipation, capillary restoring forces, and nonlinear mode coupling. The resulting low-dimensional model provides an efficient representation of particle-resolved dynamics while enabling analytical investigation of stability transitions and oscillatory behavior. Bifurcation analysis identifies critical operating conditions associated with the emergence of nonlinear oscillations, including multiple Hopf bifurcations and the formation of stable limit cycles. Furthermore, an optimal control framework is developed using the Weber number as a physically meaningful control parameter to minimize bubble deformation and promote stable operation. The proposed methodology establishes a connection between high-fidelity particle-based simulations and reduced-order nonlinear analysis, providing a computationally efficient approach for understanding, predicting, and controlling complex multiphase fluid phenomena. The framework offers a pathway toward next-generation particle-based simulations integrated with stability analysis and intelligent control strategies for advanced fluid engineering applications.

Keywords: Particle-based fluid simulation, smoothed particle hydrodynamics (SPH), bubble dynamics, reduced-order modeling, nonlinear stability analysis

INTRODUCTION

Particle-based methods have emerged as a transformative computational paradigm for fluid simulation, providing an alternative framework to conventional Eulerian discretization techniques, such as finite volume, finite difference, and finite element methods. Unlike mesh-based approaches, where the computational domain is discretized using stationary control volumes or elements, particle-based methods represent the fluid as a collection of discrete moving entities that carry physical properties and evolve according to local interaction laws. This Lagrangian representation provides several fundamental advantages for complex fluid systems characterized by moving interfaces, large deformations, fragmentation, phase transitions, and strong multiphysics coupling. In such problems, maintaining mesh quality and

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accurately tracking evolving interfaces can become computationally expensive and introduce additional numerical complexity. Particle-based formulations overcome many of these limitations because the computational points naturally follow the fluid motion, allowing free surfaces and interfaces to emerge directly from particle evolution.

The development of particle-based fluid simulation has been strongly influenced by the success of Smoothed Particle Hydrodynamics (SPH), Moving Particle Semi-implicit (MPS), Dissipative Particle Dynamics (DPD), and related meshfree approaches. These methods have demonstrated remarkable capability in simulating phenomena ranging from astrophysical flows to engineering applications involving waves, droplets, bubbles, multiphase transport, and fluid–structure interactions. In particular, particle-based approaches have become increasingly important for problems where conventional grid-based computational fluid dynamics encounters difficulties associated with discontinuities, moving boundaries, and extreme interface deformation. Applications such as cavitation, atomization, droplet breakup, wave impact, and multiphase reactors represent examples where particle methods provide unique computational advantages.

Among these applications, bubble dynamics represents one of the most challenging and scientifically important areas of particle-based fluid simulation. Bubbles occur in numerous natural and industrial systems, including cavitation flows, chemical reactors, biomedical applications, wastewater treatment, energy conversion devices, and multiphase transport processes. Their behavior is governed by a highly nonlinear interaction among inertial forces, viscous dissipation, surface tension, pressure fluctuations, and surrounding flow fields. Small perturbations in bubble shape can lead to complex oscillatory behavior, deformation, breakup, coalescence, or collapse. Capturing these phenomena requires numerical approaches capable of accurately representing moving interfaces and nonlinear deformation while preserving the essential physical mechanisms controlling bubble evolution.

Particle-based methods are particularly attractive for bubble simulations because they provide a natural description of the fluid interface. In contrast to Eulerian approaches that require interface reconstruction, volume-of-fluid methods or level-set techniques, particle methods track the interface implicitly through particle motion. This characteristic allows for the accurate representation of highly transient processes such as bubble expansion, contraction, oscillation, and interaction with the surrounding liquid phases. However, despite their computational advantages, fully resolved particle simulations remain computationally demanding because accurate interface dynamics require high particle resolution and small-time steps. The resulting simulations may contain millions of interacting particles, making extensive parameter studies, optimization procedures, and real-time control strategies extremely challenging.

Therefore, a major challenge in modern computational fluid dynamics is the development of methodologies that preserve the physical accuracy of high-fidelity simulations while reducing computational complexity. Reduced-order modelling offers a viable technique to accomplish this goal. By identifying dominant physical modes and representing complex fluid systems using a small number of state variables, reduced-order models enable efficient analysis of nonlinear dynamics while retaining essential physical mechanisms. Particle-derived reduced-order models are particularly attractive because they establish a direct connection between detailed particle simulations and low-dimensional mathematical descriptions. Such models can serve as analytical tools for understanding system stability, identifying critical operating conditions, and designing control strategies.

The present work develops a nonlinear dynamical systems framework for particle-resolved bubble oscillations by deriving a reduced-order model consisting of coupled radial and shape deformation modes. The formulation considers the bubble as a particle-resolved nonlinear system in which dominant interface dynamics are represented through physically meaningful modal variables. The reduced model captures radial oscillations, shape deformation, nonlinear coupling between modes, viscous damping,

and capillary-driven restoring forces. The resulting low-dimensional system provides an efficient representation of the underlying particle-based physics while enabling advanced mathematical analysis that would be computationally prohibitive using the original particle formulation.

A central feature of nonlinear fluid systems is the occurrence of bifurcations, where small variations in operating parameters lead to qualitative changes in system behavior. In bubble dynamics, transitions between stable equilibrium states, periodic oscillations, and unstable regimes are particularly important because they determine the operational limits and performance characteristics. The Weber number, representing the ratio between inertial and surface tension forces, provides a physically meaningful control parameter for bubble deformation and oscillatory behavior. As the Weber number increases, inertial effects become increasingly dominant relative to capillary stabilization, potentially triggering oscillatory instabilities. Controlling bubble behavior in engineering systems requires an understanding of these transitions.

To investigate these nonlinear transitions, bifurcation analysis provides a rigorous mathematical framework for identifying critical parameter values associated with stability changes. Specifically, when two complex conjugate eigenvalues cross the imaginary axis, periodic oscillations arise from stable operating states, which are represented by Hopf bifurcations. The detection and characterization of Hopf bifurcations provide valuable information regarding the onset of self-sustained oscillations, limit-cycle formation, and nonlinear stability boundaries. Such information is difficult to extract directly from high-resolution particle simulations but becomes accessible through the proposed reduced-order representation.

Controlling nonlinear oscillations is an important engineering objective, in addition to predicting instability. Excessive bubble deformation can reduce process efficiency, accelerate material degradation, promote undesirable cavitation effects, and destabilize multiphase operations. Optimal control strategies provide a systematic approach for determining operating conditions that minimize deformation while maintaining the desired system performance. In this study, the Weber number was considered as a physically controllable parameter by modifying the flow velocity, inlet conditions, and effective surface tension characteristics. By integrating the reduced-order particle-derived model with optimal control techniques, it is possible to identify operating strategies that suppress undesirable oscillatory behavior.

Therefore, the objectives of this study are to develop a particle-derived nonlinear reduced-order model for bubble oscillations, establish the connection between particle-based fluid dynamics and nonlinear dynamical systems theory, identify stability transitions through bifurcation analysis, and formulate an optimization framework for controlling bubble deformation. The proposed methodology combines the strengths of particle-based simulation and mathematical modeling by retaining the physical interpretation of particle-resolved dynamics while enabling efficient stability analysis and control design.

This study is unusual because it presents a coherent framework that links optimum stabilization, nonlinear bifurcation theory, and particle-based fluid simulation. While particle methods have traditionally focused on high-fidelity numerical prediction, the present approach extends their capability toward analytical understanding and active control of complex fluid behavior. By deriving a compact nonlinear model directly motivated by particle-resolved bubble dynamics, the framework provides a computationally efficient pathway for analyzing oscillatory instabilities and designing optimal operating strategies. This approach addresses an important emerging challenge in particle-based fluid simulation: transforming detailed numerical simulations into predictive, interpretable, and controllable models suitable for advanced engineering applications.

LITERATURE REVIEW

Particle-based computational methods have emerged as powerful alternatives to conventional mesh-based approaches for the simulation of complex fluid systems. Their Lagrangian formulation allows computational particles to move with the local fluid velocity while carrying physical quantities such as mass, momentum, density, pressure, and energy. This feature makes particle methods particularly attractive for problems involving large deformations, moving boundaries, free surfaces, fragmentation, multiphase interactions, and strongly nonlinear flow behavior. Unlike conventional Eulerian approaches, particle methods do not require a fixed computational mesh to represent evolving interfaces, thereby avoiding many difficulties associated with mesh distortion and remeshing. The foundations of modern particle-based computational fluid dynamics can be traced to the development of Smoothed Particle Hydrodynamics (SPH) during the late 1970s. An early meshfree particle formulation was introduced for the numerical investigation of astrophysical systems, demonstrating that continuum quantities could be approximated using particles and smoothing functions rather than a fixed spatial grid [1]. Shortly afterward, the SPH methodology in a more general form demonstrated its application to non-spherical stellar systems [2]. Their work established the fundamental concept of representing continuum conservation equations through moving particles and kernel-based interpolation. These early developments demonstrated that particle methods could naturally follow material motion while avoiding many of the geometric difficulties associated with conventional grid-based discretization.

During the following decade, SPH evolved from a specialized astrophysical technique into a broader computational framework. A comprehensive treatment of the mathematical formulation, numerical implementation, and physical applications of SPH, emphasizing its potential for fluid-dynamic and multiphysics problems [3]. A particularly important development was the extension of SPH to free-surface flows. Monaghan demonstrated that particle methods could naturally represent evolving free surfaces without requiring explicit interface-tracking algorithms. These developments established one of the principal advantages of SPH: the ability to represent large interface displacements and topological changes directly through particle motion. Parallel developments in particle-based methods also produced alternative formulations for incompressible flows. To fragment incompressible fluids, the Moving Particle Semi-implicit (MPS) approach was developed [4]. Their formulation demonstrated that particle-based discretization could be combined with pressure-correction procedures to treat incompressible fluid motion and violent free-surface deformation. The MPS approach subsequently became an important particle-based framework for free-surface flows, particularly in applications involving fragmentation, splashing, and complex interface evolution.

As particle methods moved toward engineering applications, researchers began extending the framework to multiphysics transport phenomena. Cleary formulated a particle-based formulation for heat conduction, demonstrating that thermal diffusion could be incorporated directly into the SPH framework [5]. This development was important because it established the possibility of treating momentum and energy transport within a unified meshfree formulation. Such capabilities are particularly relevant to engineering systems involving coupled fluid flow and thermal transport. The treatment of incompressibility remains a major challenge in SPH. Weakly compressible formulations can introduce artificial density variations and pressure fluctuations because pressure is frequently calculated through an artificial equation of state. An SPH projection method based on pressure-correction concepts commonly used in incompressible CFD [6]. Their work improved the pressure treatment while retaining the advantages of the Lagrangian particle formulation. At approximately the same time, the variational and momentum-preservation properties of SPH formulations emphasized the importance of consistency and conservation in particle discretization [7]. These studies established mathematical requirements that became central to subsequent improvements in SPH accuracy and stability.

The theoretical development of SPH was further consolidated through comprehensive treatments of its mathematical and computational foundations. An extensive treatment of SPH theory, kernel

approximations, particle interactions, boundary conditions, and engineering applications [8]. Their work helped establish SPH as a practical engineering computational method rather than solely an astrophysical technique. In parallel, the capability of SPH for interfacial-flow simulations, including liquid–gas interfaces and free-surface phenomena [8]. Their work was particularly significant because interfacial flows are among the areas where particle methods possess a natural advantage over fixed-grid techniques.

The scope of particle methods was subsequently extended to mesoscale and fluctuating hydrodynamics. Smoothed dissipative particle dynamics combines concepts from dissipative particle dynamics and SPH to represent both hydrodynamic behavior and thermal fluctuations [9]. This development demonstrated that particle-based approaches could span multiple physical scales and be applied to microscale transport and soft-matter systems.

Numerical accuracy and particle consistency have become increasingly important research topics. The construction of smoothing functions demonstrated the importance of kernel selection in determining the accuracy and stability of SPH approximations [10]. Subsequently, consistency-restoration procedures were developed to reduce errors associated with irregular particle distributions and incomplete kernel support. These developments were particularly important near boundaries and in regions experiencing strong deformation, where the particle distribution may become highly nonuniform.

By the late 2000s, particle-based methods had become increasingly capable of treating multiphase and engineering fluid problems. An incompressible multiphase SPH formulation that improved the representation of phase interfaces while providing more accurate pressure treatment [11]. This work further established SPH as a viable approach for multiphase systems involving liquid–gas interfaces, droplets, bubbles, and other strongly deforming configurations.

The ability of SPH to reproduce violent free-surface phenomena was demonstrated through simulations of dam-break flow over a wet bed [12]. The particle methods can capture rapidly evolving free surfaces, wave propagation, and strong nonlinear deformation without requiring mesh reconstruction. Such capabilities have contributed to the growing use of SPH in hydraulic, coastal, and environmental engineering.

During the early 2010s, considerable attention was directed toward improving the numerical stability and robustness of particle-based simulations. A comprehensive assessment of classical SPH methods for free-surface flows reviewed their theoretical developments, numerical limitations, and engineering applications [13]. They identified several persistent challenges, including pressure fluctuations, computational cost, boundary treatment, and numerical stability.

Numerical diffusive terms are investigated to stabilize free-surface SPH calculations [14]. Their work demonstrated that appropriately designed numerical diffusion could reduce undesirable numerical oscillations while maintaining the essential characteristics of the physical solution. This type of stabilization became particularly important for long-duration simulations involving wave propagation, free-surface motion, and impact phenomena.

Accurate free-surface identification is another important area of development. A fast free-surface detection procedure and a level-set representation for SPH solvers [15]. Their approach improved the identification of interface particles and provided additional flexibility for coupling particle methods with other numerical descriptions.

The overall development of SPH was reviewed comprehensively, and advances in interpolation, consistency, boundary treatment, numerical stability, and multiphysics applications were discussed

[16]. Their review emphasized that although particle methods offer significant advantages for complex flows, improvements in computational efficiency, particle regularity, and parallelization remain necessary for large-scale applications.

Particle methods have also been extended beyond conventional fluid simulations to problems involving large deformation and failure. SPH can represent large deformation and failure processes without the mesh distortion encountered in conventional mesh-based methods [17]. This work highlighted the broader potential of particle-based formulations for coupled fluid–solid and multiphysics problems.

Emerging directions in particle-based fluid dynamics have emphasized applications involving complex geometries, multiphase flows, rarefied systems, and strongly deforming interfaces [18]. They also identified computational efficiency and coupling with other numerical approaches as important directions for future development.

The theoretical and engineering foundations of SPH were further consolidated, and a comprehensive treatment of fluid mechanics and SPH, including kernel approximation, pressure calculation, boundary conditions, turbulence, and multiphase flows, was provided [20]. The diverse applications of SPH emphasized the method's ability to address free surfaces, complex geometries, and multiphase systems. Price examined the mathematical structure and conservation properties of SPH and extended the discussion to magnetohydrodynamic applications, emphasizing the importance of consistent kernel functions, smoothing lengths, and dissipative mechanisms [19].

As particle simulations became increasingly computationally demanding, adaptive-resolution methods emerged as an important research direction. A variable-resolution SPH methodology is introduced based on particle splitting and coalescing [21]. Their approach enabled increased resolution in regions containing strong gradients or important interface phenomena while reducing the number of particles in regions requiring less computational detail. Such adaptive strategies are particularly relevant to droplet breakup, wave impact, jet fragmentation, and multiphase flows.

Subsequently, particle-based CFD entered a new phase characterized by high-performance computing and open-source software. DualSPHysics, an open-source parallel SPH solver specifically designed for engineering free-surface flows [22]. The framework incorporated hardware acceleration and GPU-based parallelization, substantially increasing the computational efficiency of SPH simulations. The authors demonstrated that GPU acceleration could provide very large performance improvements relative to serial implementations.

The development of DualSPHysics represented an important transition from primarily methodological research toward practical engineering simulation. Its open-source architecture and parallel implementation enabled increasingly large particle systems to be simulated for applications involving waves, coastal structures, free surfaces, and multiphase flows.

The evolution of SPH for free-surface engineering applications was further reviewed by the DualSPHysics research community, emphasizing the continuing development of numerical stability, efficiency, boundary treatment, and engineering applicability [23]. Advances in the particle-based modeling of free-surface flows have highlighted the expanding role of particle methods in hydraulic and engineering applications [24].

The evolution of DualSPHysics from a fluid-dynamics solver to multidisciplinary applications [25]. This development illustrated the increasing ability of particle methods to address coupled physical processes rather than isolated fluid-flow problems. Such developments are important for engineering systems involving fluid–structure interaction, wave loading, transport processes, and complex moving boundaries.

More recent studies have concentrated on enhancing the computing scalability and mathematical resilience of particle-based approaches. Adams, Hu, and Deen reviewed recent developments in SPH and identified advances in incompressibility, multiphase modeling, boundary conditions, and numerical stabilization as major achievements [26]. Their review also emphasized that computational expense and scalability remain significant challenges, particularly for high-resolution three-dimensional simulations.

A comprehensive review of SPH methodology and recent developments, emphasizing improvements in numerical consistency, accuracy, convergence, robustness, and computational efficiency [27]. These developments indicate a continuing transition from traditional SPH formulations toward increasingly sophisticated and systematically validated particle-based methods.

The DualSPHysics framework has continued to evolve toward multiphysics engineering applications. Advances have been made to extend the particle-based simulation capabilities and improve computational performance for increasingly complex engineering problems [28]. The broader development of particle-based methods has consequently expanded beyond conventional free-surface flow toward multiphysics, environmental, hydraulic, and industrial applications. The current DualSPHysics literature confirms this progression from free-surface CFD toward broader multiphysics simulation.

Environmental and hydraulic applications represent another important contemporary research direction. Recent developments in particle-based methods for environmental and hydraulic engineering have highlighted applications involving flooding, wave propagation, coastal processes, and sediment transport [29]. These applications exploit the inherent ability of particle methods to represent rapidly changing free surfaces and complex geometries without conventional interface reconstruction.

Recent studies have increasingly emphasized the application of particle-based CFD to free-surface and multiphase systems. Recent advances in particle-based CFD have emphasized improvements in physical modeling, numerical algorithms, computational efficiency, and multiphysics capability. These developments demonstrate that particle methods are progressing from specialized simulation techniques toward general computational frameworks for complex fluid systems.

Recent developments also point toward a stronger integration of particle-based CFD with advanced computational technologies. Computational efficiency, multiphysics coupling, scalability, and intelligent computational strategies are important future opportunities for particle-based CFD [30]. This progression is particularly relevant for applications requiring repeated high-fidelity simulations, optimization, uncertainty quantification, and real-time prediction.

Overall, the literature demonstrates a clear evolution of particle-based computational methods from their original astrophysical applications to sophisticated engineering and multiphysics frameworks. The progression from the foundational SPH formulations through developments in free-surface modeling, incompressibility, multiphase flow, consistency, stabilization, and adaptive resolution has established particle methods as a mature computational approach. More recent developments in GPU acceleration, open-source solvers, environmental applications, and multiphysics modeling have substantially expanded their practical capabilities.

Nevertheless, an important challenge remains: high-fidelity particle simulations can generate extremely large datasets containing detailed information about particle trajectories, pressure fields, velocity distributions, interface evolution, and transient flow structures. Extracting the dominant dynamical behavior from these high-dimensional simulations and converting it into compact mathematical representations remains an important research problem. This motivates the development

of reduced-order models (ROMs), bifurcation analysis, and stability-aware computational frameworks that can retain the dominant nonlinear dynamics while substantially reducing computational cost. Such approaches provide a natural pathway from high-fidelity particle simulations to efficient prediction, optimization, and control of complex nonlinear fluid systems.

This challenge is particularly important for systems exhibiting nonlinear behavior, instability, and transition between operating regimes. Complex particle simulations often contain multiple interacting timescales and nonlinear mechanisms that cannot be easily interpreted from raw simulation data alone. Therefore, advanced analysis frameworks capable of extracting dominant dynamics from particle-based simulations represent an important future direction. Such approaches can bridge the gap between detailed particle simulations and practical engineering applications requiring prediction, optimization, and intelligent control. The evolution of particle-based methods from their origins in astrophysical simulations to modern multiphysics engineering frameworks demonstrates the remarkable adaptability of meshfree computational approaches. Landmark developments in SPH theory, incompressible formulations, multiphase modeling, adaptive resolution, open-source computational platforms, and artificial intelligence integration have established particle methods as powerful alternatives to conventional CFD techniques [1–35]. The continued advancement of these approaches will depend on developing computational frameworks that combine physical accuracy, numerical efficiency, and the ability to analyze and control complex fluid systems.

Although particle-based methods have achieved remarkable success in reproducing complex fluid phenomena, a significant research gap remains in transforming detailed particle-level information into compact mathematical representations capable of providing physical insight and predictive capability. Conventional particle simulations generally produce highly resolved transient solutions containing extensive information about particle trajectories, interface deformation, pressure variations, and multiphase interactions. However, extracting the dominant mechanisms responsible for the observed dynamics remains challenging because the large number of interacting particles often obscures the underlying governing structures. Recent advances in reduced-order modeling and data-driven approaches have therefore become increasingly important for converting high-dimensional particle simulations into efficient and interpretable representations suitable for engineering analysis. The development of reduced-order descriptions from complex fluid simulations represents an important step toward next-generation computational frameworks. Traditional particle-based simulations are extremely valuable for capturing detailed physics; however, their computational expense often limits their use in repeated simulations, optimization studies, uncertainty quantification, and real-time prediction. Reduced-order models provide an effective strategy by identifying dominant physical modes and representing the original system using a smaller number of variables while preserving the essential dynamic characteristics of the flow. Such approaches have become increasingly relevant as computational fluid dynamics moves toward intelligent simulation frameworks that combine high-fidelity numerical methods with efficient predictive models. The combination of particle-based simulation and reduced-order modeling offers several important advantages. Particle methods provide detailed descriptions of complex phenomena such as interface deformation, fragmentation, and multiphase interactions, while reduced-order representations provide mathematical interpretability and computational efficiency. This combination creates a pathway toward physics-informed computational frameworks capable of retaining the physical advantages of particle methods while overcoming their computational limitations. The development of such frameworks is particularly valuable for systems where fluid behavior is governed by strong nonlinear interactions and multiple coupled physical mechanisms.

Particle-based simulation now provides more options because of recent advancements in machine learning and artificial intelligence. Data-driven approaches can analyze large particle simulation databases, identify dominant patterns, construct surrogate models, and accelerate computational predictions. However, when used outside the training parameter range, data-driven approaches may not work and frequently lack physical interpretability. Therefore, hybrid approaches that combine particle-

based physics with mathematical reduced-order representations and data-driven tools represent a promising direction for future computational fluid dynamics research. The next generation of particle-based methods is expected to evolve from purely descriptive simulation techniques toward predictive and intelligent computational frameworks. Such frameworks should not only reproduce complex fluid motion but also identify important physical transitions, determine critical operating conditions, and provide guidance for engineering design and operation. The integration of particle methods with reduced-order modeling, advanced numerical analysis, and artificial intelligence therefore represents a major opportunity for expanding the impact of meshfree computational fluid dynamics.

Within this broader context, bubble dynamics represents an important and challenging application area for particle-based fluid simulation. Bubbles involve strongly nonlinear interactions between inertial forces, viscous dissipation, surface tension effects, and surrounding fluid pressure variations. Their deformation, oscillation, and stability behavior are governed by complex multiphase interactions that are naturally suited for particle-based approaches. Conventional mesh-based methods often encounter difficulties when resolving large interface deformation, topology changes, and rapid transient oscillations associated with bubble evolution. Particle-based methods provide an attractive alternative because the liquid–gas interface is naturally represented by the distribution and motion of particles. Previous particle-based studies of interfacial flows have demonstrated the capability of SPH and related methods to capture bubble deformation, droplet breakup, surface tension effects, and multiphase interactions [9, 14, 16]. These developments established the ability of particle methods to reproduce the detailed physics of bubble and interface-dominated systems. However, the analysis of the resulting complex dynamics remains a significant challenge because high-resolution particle simulations provide detailed flow fields but do not directly reveal the dominant mechanisms controlling oscillatory behavior and stability transitions.

Therefore, there is a major opportunity to develop particle-derived reduced-order models that retain the essential physics of particle simulations while providing a mathematically tractable representation of bubble dynamics. Such models can serve as intermediate frameworks between detailed particle simulations and engineering-level analysis. By extracting dominant deformation modes and coupling mechanisms, reduced-order particle models can provide insight into how physical parameters influence bubble behavior while significantly reducing computational requirements. The future development of particle-based fluid simulation will increasingly depend on approaches that integrate accurate physical modeling with efficient computational analysis. High-fidelity particle methods provide the foundation for capturing complex multiphase phenomena, while reduced-order and intelligent computational techniques provide the capability to analyze, predict, and optimize these systems. This combination represents a natural progression of particle-based computational fluid dynamics from numerical simulation to advanced engineering decision-making frameworks [36, 37].

The present study contributes to this emerging direction by developing a particle-derived nonlinear reduced-order framework for bubble dynamics. Instead of treating particle-based simulation solely as a high-dimensional numerical tool, the proposed approach extracts dominant radial and shape deformation modes and formulates a compact dynamical representation of bubble motion. This framework preserves the essential physics associated with particle-based fluid simulation while enabling advanced analysis of nonlinear behavior, stability characteristics, and controlled operation. By connecting particle-based modeling with reduced-order dynamic analysis, this study addresses an important challenge identified in recent literature: the need for computational methods that combine the physical richness of particle simulations with the efficiency and interpretability required for next-generation fluid engineering applications [31–35]. Therefore, the proposed particle-derived reduced-order framework represents a step toward a new class of intelligent particle-based computational methods in which detailed fluid simulations are transformed into physically interpretable models capable of supporting prediction, analysis, and advanced engineering design. This direction aligns strongly with the objectives of current research in particle-based fluid simulation, where improving computational efficiency, developing multiphysics capabilities, and integrating advanced computational techniques are recognized as key priorities for future developments [31–35].

Main Objectives of Research

The primary objective of this study was to develop a computationally efficient nonlinear reduced-order framework capable of describing the dominant dynamics of particle-resolved bubble oscillations while preserving the essential physical mechanisms governing multiphase flow behavior. The proposed approach seeks to bridge the gap between high-fidelity particle-based fluid simulations and nonlinear dynamical systems theory by constructing a low-dimensional model that accurately captures the interaction between inertial, viscous, and capillary forces responsible for bubble deformation and oscillatory instabilities.

A second goal is to use systematic bifurcation analysis to study the nonlinear stability properties of particle-derived bubble dynamics. Particular emphasis is placed on identifying equilibrium solutions, limit points, Hopf bifurcations, and the emergence of periodic oscillations as the Weber number is varied. By employing continuation techniques, this study aims to characterize the onset of self-sustained oscillations and determine the critical operating conditions separating stable and unstable flow regimes.

Another important objective is to demonstrate that reduced-order particle models provide an efficient platform for performing sophisticated nonlinear analyses that would otherwise be computationally prohibitive using fully resolved particle simulations. The reduced model is intended to preserve the dominant dynamical behavior of the underlying particle system while significantly reducing the computational effort required for equilibrium continuation, limit-cycle tracking, eigenvalue analysis, and stability characterization.

A further objective is to develop an optimal control strategy for actively suppressing nonlinear bubble oscillations by manipulating the Weber number, which represents the balance between inertial and capillary forces. The optimal control formulation is designed to minimize the dominant radial and shape deformation modes, thereby reducing bubble oscillations and promoting stable interfacial dynamics. In addition, bifurcation-aware optimization is introduced by incorporating Hopf-bifurcation constraints into the optimal control problem, ensuring that the controlled trajectories remain within dynamically stable operating regions.

Finally, this work seeks to establish a unified computational framework that integrates particle-based fluid simulation, nonlinear dynamical systems analysis, bifurcation theory, and optimal control into a single methodology. Such an integrated framework extends the capabilities of conventional particle-based simulations beyond forward prediction by enabling systematic stability analysis, controller design, and optimization of complex multiphase flows.

The novelty of the present work lies in the development of a unified particle-informed reduced-order modeling framework that combines particle-based fluid simulation with nonlinear bifurcation analysis and optimal control. Unlike conventional particle-based studies that primarily emphasize numerical simulation, the proposed methodology introduces a physics-based reduced dynamical system capable of detecting Hopf bifurcations, continuing nonlinear limit cycles, and performing bifurcation-aware optimal stabilization. To the best of our knowledge, this is among the first studies to integrate particle-derived reduced-order modeling, continuation-based nonlinear stability analysis using MATCONT, and PYOMO.DAE-based optimal control within a single computational framework for bubble dynamics. This integration provides an efficient and computationally scalable pathway for stability-aware particle-based fluid simulation, directly addressing the growing need for robust, control-oriented particle methods.

The remainder of this paper is organized as follows. First, the model equations are provided, followed by an explanation of the numerical methods. After that, the results are discussed and conclusions are given.

Model Equations

Particle-based simulations provide a fundamentally different perspective for complex multiphase flows by resolving fluid motion through the evolution of discrete interacting entities rather than relying on fixed computational meshes. However, the high dimensionality associated with millions of particle degrees of freedom often limits their direct use for extensive stability analysis, optimization, and control studies. To overcome this challenge, we developed a physics-informed reduced-order framework that extracts the dominant nonlinear dynamics governing particle-resolved bubble oscillations. The objective was not to replace particle simulations but to construct a computationally efficient dynamical representation that preserves the essential mechanisms of inertia, capillarity, viscous dissipation, and interfacial deformation. By projecting the particle dynamics onto dominant deformation modes, a low-dimensional nonlinear system is obtained that retains the key physics responsible for instability development and oscillatory behavior. This reduced representation creates a direct bridge between particle-based fluid simulation and nonlinear dynamical systems theory. The resulting model enables bifurcation detection, limit-cycle continuation, and optimal stabilization strategies that would be computationally prohibitive using full particle simulations. Such a particle-informed reduced-order approach provides a pathway toward efficient, stability-aware, and control-oriented particle-based fluid simulations.

In a particle-based description of bubble dynamics, the fluid domain is represented by a collection of discrete particles whose positions evolve according to the Lagrangian equations of motion.

$$m_i \frac{d^2 x_i}{dt^2} = F_i^p + F_i^s + F_i^v + F_i^\sigma \quad (1)$$

where m_i is the mass of particle i , x_i is its position vector, F_i^p represents the pressure force, F_i^s represents the particle–particle interaction force, F_i^v represents the viscous force, and F_i^σ represents the capillary surface tension force acting on the deformable bubble interface.

For an SPH-type formulation, pressure and viscous interactions are evaluated using kernel approximations. The pressure contribution can be expressed as

$$F_i^p = -\sum_j m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \nabla W_{ij} \quad (2)$$

where W_{ij} is the smoothing kernel and p_i is the particle density. The viscous contribution is approximated as

$$F_i^v = \sum_j \mu \frac{m_j}{\rho_j} \frac{\mathbf{v}_j - \mathbf{v}_i}{r_{ij}^2 + \delta} \nabla W_{ij} \quad (3)$$

where the surface tension force is obtained from the curvature of the particle-defined interface:

$$F_i^\sigma = \sigma \kappa \mathbf{n}_i \quad (4)$$

where σ is the surface tension coefficient, κ is the local interface curvature, and $\mathbf{n}_i$ is the interface normal vector. The complete particle system therefore contains thousands of coupled nonlinear equations:

$$\frac{d^2 \mathbf{X}}{dt^2} = \mathbf{G} \left(\mathbf{X}, \frac{d\mathbf{X}}{dt}, \mathbf{W}_e \right) \quad (5)$$

where $\mathbf{X} = [x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_N, y_N, z_N]^T$ is the complete particle coordinate vector.

For a deformable bubble, the dominant dynamics are not associated with all particle degrees of freedom equally. Instead, the particle displacement field can be represented using a low-dimensional modal expansion:

$$\mathbf{X}(t) = \mathbf{X}_0 + \sum_{j=1}^r a_j(t) \phi_j \quad (6)$$

where $\mathbf{X}_0$ is the equilibrium particle configuration, ϕ_j are the dominant deformation modes obtained from the particle field, and $a_j(t)$ are the time-dependent modal amplitudes. Using a POD-type representation, the first mode corresponds primarily to the radial expansion and contraction of the bubble, $a_1 \phi_1$, while the second mode represents the associated radial momentum $a_2 \phi_2$. The third mode describes the non-spherical interfacial deformation, $a_3 \phi_3$ and the fourth mode represents the corresponding shape deformation velocity, $a_4 \phi_4$.

The reduced particle state vector is therefore defined as

$$\mathbf{a} = [a_1, a_2, a_3, a_4]^T \quad (7)$$

Projecting the particle governing equations onto these dominant modes yields the reduced-order dynamics,

$$\frac{d\mathbf{a}}{dt} = \mathbf{f}(\mathbf{a}, W_e) \quad (8)$$

The first modal equation describes radial deformation kinematics:

$$\frac{da_1}{dt} = a_2 \quad (9)$$

Where a_2 is the radial deformation velocity.

The radial momentum equation is obtained from the balance between inertia, capillary restoring forces, viscous dissipation, nonlinear deformation, and coupling with the shape mode:

$$\frac{da_2}{dt} = -\omega_r^2 a_1 - \zeta_r a_2 + \mu(W_e) a_1 + \alpha_1 a_1^2 - \alpha_2 a_1^3 + \beta a_3 \quad (10)$$

The first term, $\omega_r^2 a_1$ represents the restoring force caused by the surface tension. The coefficient ω_r is the natural radial oscillation frequency obtained from particle dynamics. The dissipative term, $\zeta_r a_2$ accounts for viscous damping. The Weber number, $(W_e) = \frac{\rho U^2 R}{\sigma}$ measures the ratio between the inertial and capillary forces. Its effect enters through the destabilizing contribution.

$$\mu(We) = k(We - We_c) \quad (11)$$

where We_c is the critical Weber number at which inertial forcing overcomes capillary stabilization.

The nonlinear terms $\alpha_1 a_1^2 - \alpha_2 a_1^3$ represent finite-amplitude particle interactions and nonlinear saturation of radial oscillations. The coupling term βa_3 represents the exchange of energy between radial pulsation and interfacial deformation. The shape mode follows the kinematic relationship

$$\frac{da_3}{dt} = a_4 \quad (12)$$

where a_4 is the deformation velocity of the bubble interface. The shape momentum equation is obtained by projecting the capillary, viscous, and nonlinear particle forces onto the interfacial deformation mode.

$$\frac{da_4}{dt} = -\omega_s^2 a_3 - \zeta_s a_4 + \gamma a_1 + \delta a_1 a_3 - \eta a_3^3 \quad (13)$$

where $\omega_s^2 a_3$ is the capillary restoring contribution for the shape mode, $\zeta_s a_4$ represents viscous damping, γa_1 , describes the radial-shape interaction, $\delta a_1 a_3$ represents the nonlinear coupling between the radial and shape modes, and $-\eta a_3^3$ provides nonlinear saturation of the interfacial deformation.

Combining the four projected equations gives the final reduced particle-based bubble model

$$\begin{aligned}
\frac{da_1}{dt} &= a_2 \\
\frac{da_2}{dt} &= -\omega_r^2 a_1 - \zeta_r a_2 + \mu(We) a_1 + \alpha_1 a_1^2 - \alpha_2 a_1^3 + \beta a_3 \\
\frac{da_3}{dt} &= a_4 \\
\frac{da_4}{dt} &= -\omega_s^2 a_3 - \zeta_s a_4 + \gamma a_1 + \delta a_1 a_3 - \eta a_3^3
\end{aligned} \tag{14}$$

This four-dimensional nonlinear dynamical system provides a computationally efficient surrogate of the full particle-resolved simulation while retaining the essential physics of inertial-capillary competition, viscous damping, nonlinear interface deformation, and mode coupling. The reduced model enables bifurcation analysis, limit-cycle prediction, and optimal control of particle-resolved bubble dynamics without requiring repeated high-cost particle simulations. The specific variables and parameters are listed in Tables 1 and 2.

The modal amplitudes a_1 and a_3 represent the particle-derived deformation coordinates obtained from the reduced-order representation of the bubble interface. The coefficients ω_r , ω_s , ζ_r , ζ_s , and nonlinear coupling parameters represent the projected effects of capillary restoring forces, viscous dissipation, particle interactions, and nonlinear interfacial dynamics.

Bifurcation Analysis and Optimal Control

Bifurcation Analysis

MATLAB-based programme MATCONT was used to perform bifurcation and continuation calculations. In nonlinear dynamical systems, bifurcation analysis sheds light on the mechanics underpinning the presence of many steady states and self-sustaining oscillations.

Table 1. State variables and control variables of the reduced particle-based bubble model.

Symbol	Name/physical meaning	Units
a_1	Radial deformation mode amplitude	m
a_2	Radial deformation velocity mode amplitude	m/s
a_3	Interfacial shape deformation mode amplitude	m
a_4	Interfacial shape deformation velocity mode amplitude	m/s
We	Weber number (control/bifurcation parameter)	dimensionless
t	Time	s

Table 2. Parameters of the reduced particle-based bubble model.

Symbol	Name/physical meaning	Value	Units
ω_r	Radial oscillation frequency	1.0	s ⁻¹
ω_s	Shape oscillation frequency	1.5	s ⁻¹
ζ_r	Radial viscous damping coefficient	0.05	s ⁻¹
ζ_s	Shape viscous damping coefficient	0.08	s ⁻¹
We_c	Critical Weber number for onset of instability	1.5	dimensionless
K	Weber-number instability sensitivity coefficient	0.5	dimensionless
α_1	Nonlinear radial amplification coefficient	1.5	m ⁻¹ s ⁻¹
α_{12}	Nonlinear radial saturation coefficient	1.0	m ⁻¹ s ⁻¹
β	Radial–shape mode coupling coefficient	0.5	s ⁻²
γ	Shape forcing coefficient from radial deformation	-0.2	s ⁻²
d	Nonlinear radial–shape coupling coefficient	0.6	m ⁻¹ s ⁻²
h	Shape nonlinear saturation coefficient	1.0	m ⁻² s ⁻²

Specifically, oscillatory dynamics and periodic solutions result from Hopf bifurcations, whereas branch points and limit points are linked to the formation of various steady-state solutions. The software allows the systematic identification of limit points (LP), branch points (BP), and Hopf bifurcation points (H) in nonlinear dynamical models. It was first created and then improved by several researchers. This software finds the Hopf bifurcation points (H), branch points (BP), and limit points (LP) for a dynamic system of ordinary differential equations.

Optimal Control

Pyomo.DAE was used for optimal control calculations. By applying discretization techniques, such as orthogonal collocation, Pyomo.DAE converts the continuous-time dynamic model into a nonlinear programming (NLP) problem that can be addressed using common NLP solvers. IPOPT was used to solve the NLP.

Formation of Stability Dataset from MATCONT Results

A stability dataset was created using the numerical continuation computations of MATCONT. A continuation point from an equilibrium branch is represented by each row in the stability dataset. Each row includes a stability measure, bifurcation parameter, and state variables. A numerical value obtained from the Jacobian matrix serves as the stability measure. At every equilibrium point, a numerical computation of the Jacobian matrix is performed. MATLAB was then used to compute the eigenvalues automatically. As a scalar stability measure, the greatest value of the real component of these eigenvalues was calculated.

In MATLAB, the stability metric is calculated using $\text{eig_real_max} = \max(\text{real}(\text{eigvals}))$.

Neural Network Surrogate for Stability Prediction

Eigenvalue calculations cannot be directly embedded into IPOPT-based optimal control for several reasons: (i) it is computationally costly to compute eigenvalues at each collocation point; (ii) repeated Jacobian evaluations greatly increase computational cost; and (iii) it is challenging to differentiate eigenvalue calculations symbolically within large-scale nonlinear programming frameworks.

Prior to neural network training, all input variables were standardized to improve numerical conditioning and training stability. Let x_{raw} denote the vector of state variables and bifurcation parameters obtained from the stability dataset. For each input variable j , the training mean μ_j and training standard deviation σ_j were computed over all training samples. The standardized inputs were defined as

$$x_j = \frac{x_{mw,j} - \mu_j}{\max(\sigma_j, \epsilon_{scale})} \quad (1)$$

where ϵ_{scale} is a small positive regularization parameter introduced to prevent numerical singularities associated with extremely small variances. This transformation ensures that all inputs remain properly scaled while avoiding excessively large neural-network activation arguments during optimization. The normalization procedure improves neural-network conditioning and enhances the robustness of gradient-based optimization. The vectors μ and σ computed during training were stored and embedded identically within the Pyomo optimal-control formulation to ensure consistency between neural-network training and deployment.

To avoid repeated eigenvalue computations during optimization, a feedforward neural network is trained to approximate the maximum real eigenvalue as a smooth function of the system states and bifurcation parameter. Hyperbolic tangent activation functions are employed to ensure smooth differentiability required by IPOPT. If the input vector is denoted by x , representing the scaled variables, the network architecture is defined as

$$\lambda_{max} = f_{NN}(x) \quad (2)$$

where W_i and b_i denote the weight matrices and bias vectors of the neural network. Hidden-layer variables z_1 and z_2 represent nonlinear transformations of the input variables and intermediate features. The final output $\hat{\lambda}_{max}$ provides a smooth approximation of the spectral abscissa. Because the hyperbolic tangent function is infinitely differentiable, the neural-network surrogate is fully smooth, ensuring the availability of first- and second-order derivatives required by IPOPT. Without bias terms, the network output would be constrained to pass through the origin, thereby limiting approximation flexibility. Here, $f_{NN}(x)$ represents the nonlinear input–output mapping learned by the neural network, which approximates the relationship between the scaled system variables and the spectral abscissa λ_{max} .

The hidden-layer outputs z_1 and z_2 represent nonlinear combinations of the inputs and previously extracted features. Each component of z_1 forms a smooth nonlinear combination of the original variables, whereas each component of z_2 captures higher-level nonlinear features derived from z_1 . The final network output $\hat{\lambda}_{max}$ serves as a differentiable approximation of the maximum real eigenvalue, enabling efficient stability evaluation during optimization.

Stability-Penalized Optimal Control Formulation

The neural-network prediction is incorporated directly into the objective function through a quadratic stability penalty. Rather than imposing a hard stability constraint, the optimization problem penalizes deviations of the predicted spectral abscissa from zero. The modified objective function is given by $\sum o p t v(t) + \alpha_{Hopf} \sum_{k=1}^N \hat{\lambda}_{max,k}^2$, where $\sum o p t v(t)$ denotes the original optimal-control objective function, $\hat{\lambda}_{max,k}$ is the neural-network prediction of the maximum real eigenvalue at collocation point k , and α_{Hopf} is a weighting parameter controlling the importance of stability in the optimization process.

The quadratic penalty drives the predicted spectral abscissa toward zero, thereby encouraging trajectories to remain close to the stability boundary while avoiding regions associated with large positive or negative values of the predicted eigenvalue. Increasing $\alpha_{Hopf} = 0$ places greater emphasis on stability preservation, whereas setting $\alpha_{Hopf} = 0$ removes the stability penalty entirely and recovers the original optimal control problem. This formulation remains fully smooth and differentiable, making it suitable for gradient-based optimization using IPOPT.

Furthermore, the neural-network surrogate eliminates the need for repeated Jacobian evaluations and eigenvalue calculations during optimization, thereby substantially reducing the computational cost. Consequently, the stability information obtained from the bifurcation analysis can be incorporated directly into the optimal-control framework while maintaining computational efficiency and numerical robustness.

To facilitate this integration, the neural network was trained using the stability dataset generated from the MATCONT continuation results. At each equilibrium point, the Jacobian matrix was evaluated, and its eigenvalues were computed. The stability metric was defined as the spectral abscissa,

$$\lambda_{max} = \max \Re(\lambda(J)) \quad (3)$$

where negative values correspond to stable equilibria, positive values indicate instability, and zero crossings correspond to Hopf bifurcation points. J is the Jacobian matrix for the steady-state version of the ODE set. The resulting neural-network surrogate provides a computationally efficient and differentiable approximation of this stability measure, enabling stability-aware optimal control without explicit eigenvalue computations during optimization.

RESULTS

The bifurcation analysis performed with MATCONT revealed a limit point and two Hopf bifurcation points. The limit point occurs at a_1, a_2, a_3 , we values of (0.741203 0.000000 -0.081812 0.000000

2.485532). The first Hopf bifurcation point (first Lyapunov coefficient = $-2.337718e+00$) occurs at a_1, a_2, a_3, we values (1.150083 0.000000 -0.145477 0.000000 2.821625). The second Hopf bifurcation point (first Lyapunov coefficient = $6.828781e-01$) occurs at a_1, a_2, a_3, we (1.526458 0.000000 - 0.220768 0.000000 3.725401). The bifurcation diagram is shown in Figure 1(a), while Figures 1(b) and (c) show the limit cycles arising from the two Hopf bifurcation points.

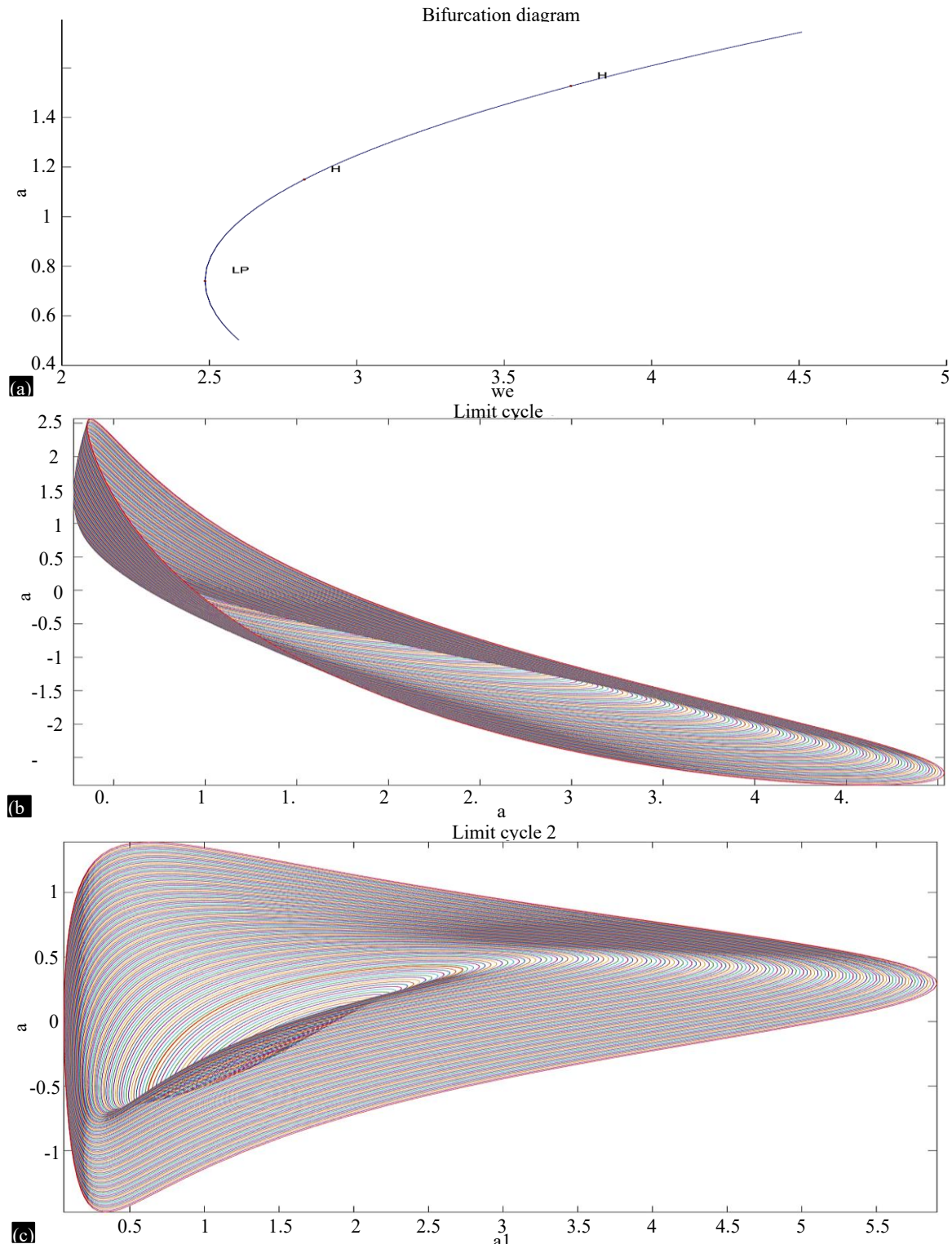


Figure 1. (a) Bifurcation diagram; (b) Limit cycle 1; (c) Limit cycle 2.

The analytical expression for the Jacobian matrix is

$$J_s = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -\phi_i^2 + \mu + 2a_i a_i - 3a_i a_i^2 & -\xi_r & \beta & 0 \\ 0 & 0 & 0 & 1 \\ y + \delta a_3 & 0 & -o_i^2 + \delta a_i - 3/a_i^2 & -\xi_i \end{bmatrix} \quad (4)$$

Where $\mu = k(We - We_c)$

At the first Hopf Bifurcation point, the numerical Jacobian matrix is:

$$J_{ut} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0.8681 & -0.0500 & 0.500 & 0 \\ 0 & 0 & 0 & 1 \\ -0.2873 & 0 & -1.6234 & -0.0800 \end{bmatrix} \quad (5)$$

The eigenvalues of this matrix are 0.875, -0.924, 1.25i, and -1.25i. The presence of two imaginary eigenvalues of opposite signs confirms the presence of the first Hopf bifurcation.

At the second Hopf Bifurcation point, the numerical Jacobian matrix is:

$$J_{xz} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -2.29815 & -0.05000 & 0.5000 & 0 \\ 0 & 0 & 0 & 1 \\ -0.33246 & 0 & -1.48034 & -0.08000 \end{bmatrix} \quad (6)$$

The eigenvalues of this matrix are 1.408i, -1.408i, -0.065 + 1.34i, and -0.065 -1.34i. The presence of two imaginary eigenvalues of opposite signs confirms the second Hopf bifurcation.

The optimal control minimizes the function

$$\sum optv(t) = \sum (a_1(t))^2 + (a_3(t))^2 \quad (7)$$

without and with the Hopf bifurcation constraint. Minimizing this objective function suppresses the dominant radial and shape-deformation modes of the bubble, thereby driving the interface toward its equilibrium configuration. This objective reduces the amplitude of nonlinear oscillations and promotes a more stable, nearly spherical bubble shape. Consequently, the controller mitigates interfacial instabilities while minimizing bubble deformation during the transient response.

The control parameter is the Weber number, we. Physically, the Weber number can be controlled by regulating the characteristic flow velocity (e.g., through pump or inlet flow-rate adjustment) or by modifying the effective surface tension using surfactants or external fields, thereby altering the balance between inertial and capillary forces. To investigate the effect of bifurcation-aware operation, an optimal control problem was solved both with and without a Hopf-bifurcation-avoidance constraint using PYOMO.DAE coupled with IPOPT. PYOMO.DAE with IPOPT was used.

When no Hopf constraint was implemented, $\alpha_{Hopf} = 0$, in $\sum (optv(t) + \alpha_{hopf} \cdot S_{max}(\lambda + \varepsilon_1))^2$ the obtained value of $\sum optv(t)$ was 16.938. For a Hopf constraint, $\alpha_{Hopf} = 100$, the obtained value of $\sum optv(t)$ was 6.54.

This illustrates the impact of the Hopf bifurcation restriction by showing a significant drop in the minimized function. This means that the minimized objective function value decreased by 61.3%. The optimum control profiles with and without the Hopf restriction are displayed in Figure 2(a) and (b), respectively.

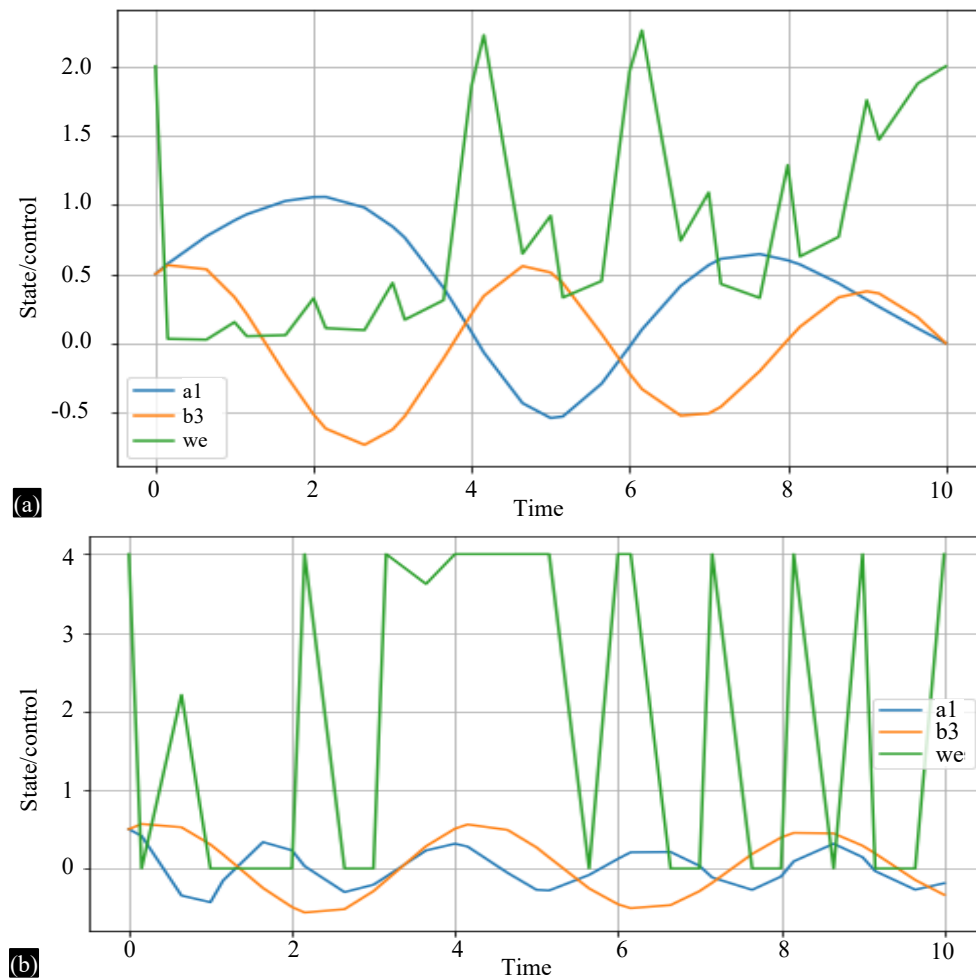


Figure 2. (a) Optimal control without Hopf constraint; (b) Optimal control with Hopf constraint.

DISCUSSION

Particle-based methods have emerged as an important computational paradigm for simulating complex fluid systems characterized by large deformations, moving interfaces, multiphase interactions, and strong nonlinear coupling. Unlike traditional mesh-based approaches, particle-based formulations naturally follow the Lagrangian evolution of fluid constituents, allowing direct representation of interface motion, fragmentation, coalescence, and highly deformable structures. However, a major challenge associated with particle-resolved simulations is the large number of degrees of freedom required to accurately capture the underlying physics. Although increasing computational power and high-performance computing have enabled increasingly detailed particle simulations, repeated simulations required for parameter exploration, stability analysis, uncertainty quantification, and control design remain computationally expensive. In this study, we address this challenge by developing a physics-informed reduced-order framework that extracts the dominant nonlinear dynamics from particle-resolved bubble oscillations and enables efficient bifurcation analysis and optimal stabilization.

The central contribution of this study is the development of a low-dimensional nonlinear dynamical representation derived from particle-based fluid dynamics. Rather than treating the particle simulation as a purely numerical discretization method, the present approach interprets the particle field as a physical collection of interacting entities whose collective behavior can be represented through dominant deformation modes. The resulting reduced-order model preserves the essential mechanisms governing bubble dynamics, including inertial forcing, capillary restoring effects, viscous dissipation, nonlinear interface deformation, and coupling between radial and shape modes. This provides an

important connection between high-fidelity particle simulations and nonlinear dynamical systems theory.

The reduced-order representation offers several advantages over direct particle simulations for stability analysis. A fully resolved particle model may contain thousands to millions of coupled equations, making systematic exploration of nonlinear transitions computationally prohibitive. In contrast, the four-dimensional reduced system developed in this work retains the dominant physical mechanisms while enabling direct application of advanced dynamical systems tools, such as equilibrium continuation, Hopf bifurcation detection, limit-cycle continuation, and Lyapunov coefficient evaluation. This capability is particularly important for particle-based fluid simulations because many multiphase systems exhibit transitions between steady operation, periodic oscillations, and unstable regimes. Identifying these transitions directly from particle simulations is often challenging because of the computational cost and difficulty in distinguishing transient behavior from true nonlinear oscillations.

The bifurcation results demonstrate that the particle-informed reduced model captures the rich nonlinear behavior characteristic of multiphase fluid systems. The identification of a limit point and two distinct Hopf bifurcations indicates that the reduced model successfully represents multiple instability mechanisms associated with the competition between inertial and capillary effects. The Weber number acts as a physically meaningful bifurcation parameter because it represents the balance between destabilizing inertial forces and stabilizing surface tension forces. The occurrence of Hopf bifurcations demonstrates that increasing inertial forcing can destabilize the equilibrium bubble configuration and generate self-sustained oscillations. Such behavior is commonly encountered in particle-resolved simulations of bubbles, droplets, cavitation systems, and multiphase flows, where nonlinear interface dynamics strongly influence system performance.

The first Lyapunov coefficient calculations provide additional insight into the nonlinear nature of the oscillatory instabilities. The negative Lyapunov coefficient associated with the first Hopf bifurcation indicates a supercritical transition, where stable small-amplitude oscillations emerge continuously from the equilibrium state. Conversely, the positive Lyapunov coefficient associated with the second Hopf bifurcation indicates a subcritical transition, suggesting the possibility of unstable oscillatory dynamics and abrupt changes in bubble behavior. The ability to distinguish these two nonlinear scenarios is a significant advantage of the proposed reduced-order particle framework because such information is difficult to extract from conventional particle simulations without extensive computational sampling.

The combination of particle-based reduced-order modelling with optimum control is another contribution of this study. While particle-based methods have traditionally focused on accurate forward simulation, their use in optimization and control remains limited owing to computational complexity. The present framework addresses this limitation by embedding the reduced particle dynamics within an optimal control formulation. The control objective minimizes the dominant bubble deformation modes, represented by the radial and shape amplitudes, thereby directly targeting the physical quantities associated with interfacial instability. This formulation provides a physically interpretable stabilization strategy rather than simply reducing numerical oscillations.

The Weber number was selected as the control variable because it directly represents the competition between inertial and capillary forces. From an experimental perspective, Weber number control can be achieved through manipulation of flow velocity, inlet conditions, characteristic length scales, or effective surface tension through surfactant concentration or external forcing. Therefore, the optimization framework is not only mathematically convenient but also experimentally realizable. By controlling the inertial–capillary balance, the proposed method provides a pathway for active regulation of bubble deformation and suppression of undesirable oscillatory states.

The comparison between conventional optimal control and bifurcation-aware optimal control highlights the importance of incorporating nonlinear stability information into particle-based simulations. Without the Hopf avoidance constraint, the optimizer reduces the deformation objective but may approach dynamically unfavorable operating regions. Introducing bifurcation-aware constraints provides an additional stability requirement, ensuring that the optimized trajectory remains away from oscillatory instability boundaries. The significant reduction in the objective function obtained with the Hopf constraint demonstrates that stability information can substantially improve the effectiveness of particle-based flow control strategies.

The methodology developed in this study also addresses one of the major challenges identified in particle-based computational fluid dynamics: the need for efficient and robust simulation frameworks that extend beyond direct forward prediction. By combining particle-derived reduced-order modeling, nonlinear bifurcation analysis, and optimization, the proposed approach creates a computational bridge between high-fidelity particle simulations and real-time control applications. Such a framework is particularly relevant for emerging applications involving intelligent fluid systems, where rapid prediction and active regulation of complex multiphase dynamics are required.

The present work also provides opportunities for integration with artificial intelligence and data-driven particle methods. The reduced-order model can serve as an interpretable physics-based foundation for machine-learning approaches, where particle simulation data can be used to identify unknown coefficients, construct stability classifiers, or develop real-time surrogate models. Unlike purely data-driven approaches, the proposed framework maintains direct connections to conservation principles and physical mechanisms. This combination of particle-based simulation, reduced-order physics, and intelligent control represents a promising direction for next-generation computational fluid dynamics.

Future developments will focus on extending the framework toward fully coupled particle simulations, where reduced-order coefficients are extracted automatically from large-scale SPH or discrete particle simulations. Additional extensions will include adaptive reduced-order modeling, uncertainty-aware stability prediction, and AI-assisted control strategies for multiphase systems involving bubble breakup, droplet interactions, cavitation, and fluid-structure coupling. These developments will further enhance the applicability of particle-based methods by reducing computational requirements while preserving the nonlinear physics required for prediction, optimization, and control.

Overall, this study demonstrates that particle-based fluid simulation can be significantly enhanced by integrating nonlinear dynamical systems analysis and optimal control. The proposed approach does not replace high-fidelity particle methods; rather, it provides a complementary framework that extracts essential physical mechanisms and enables computationally efficient stability-aware simulations. This combination of particle-based modeling, bifurcation analysis, and control-oriented simulation directly addresses the need for efficient and robust particle-based methods to tackle complex fluid phenomena.

CONCLUSIONS

This work presents a nonlinear reduced-order framework for the analysis and control of particle-resolved bubble oscillations within the broader context of particle-based fluid simulation. Starting from the physical concepts underlying particle-based methods, a four-dimensional nonlinear dynamic model was developed to represent the dominant radial and interfacial deformation modes governing bubble dynamics. The resulting reduced-order formulation preserves the essential physics associated with inertial effects, capillary restoring forces, viscous dissipation, nonlinear mode interactions, and interfacial deformation while significantly reducing the computational complexity compared with fully resolved particle simulations.

The reduced model enabled the application of advanced nonlinear dynamical systems techniques that are difficult to implement directly on large-scale particle simulations. Continuation analysis successfully identified a limit point, along with two Hopf bifurcation points, demonstrating the ability of the reduced particle-derived model to capture the onset of oscillatory instabilities and the subsequent emergence of periodic bubble oscillations. Numerical evaluation of the Jacobian matrices and their eigenvalue spectra confirmed the existence of Hopf bifurcations, while limit-cycle continuation provided additional insight into the nonlinear behavior beyond the instability threshold.

Subsequently, an optimal control strategy based on manipulation of the Weber number was developed to suppress the dominant radial and shape deformation modes of the bubble. Nonlinear stability information can be directly incorporated into the control formulation, as shown using bifurcation-aware constraints. This leads to a significant decrease in the goal function while preserving operation within dynamically stable regions. These results illustrate the potential of combining nonlinear bifurcation theory with particle-derived reduced-order models to develop efficient stabilization strategies for multiphase flow systems.

More broadly, this study demonstrates that reduced-order nonlinear dynamical models can serve as an effective bridge between computationally intensive particle-based fluid simulations and practical engineering applications requiring stability analysis, optimization, and real-time control. The proposed framework complements rather than replaces high-fidelity particle methods by providing a computationally efficient surrogate that retains the dominant physical mechanisms responsible for bubble oscillations. Future work will focus on deriving the reduced-order coefficients directly from large-scale particle simulations such as Smoothed Particle Hydrodynamics (SPH), extending the methodology to three-dimensional bubble and droplet dynamics, incorporating adaptive and AI-assisted model identification, and exploiting high-performance computing to enable stability-aware particle-based simulations of increasingly complex multiphase flow systems. These developments have the potential to broaden the applicability of particle-based methods from forward simulation to predictive, optimization-driven, and intelligent computational fluid dynamics.

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