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SPHinXsys: An open-source meshless, multi-resolution and multi-physics library

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ABSTRACT

In this paper, we present an open-source meshless, multi-resolution and multi-physics library: SPHinXsys (pronunciation: s'finksis) which is an acronym for Smoothed Particle Hydrodynamics (SPH) for industrial compleX systems. It aims at modeling coupled multi-physics industrial dynamic systems including fluids, solids, multi-body dynamics and beyond in a multi-resolution unified SPH framework. The code presently (Version: 0.2.0) includes fluid dynamics, solid dynamics, thermal and mass diffusion, electro-chemical reaction, fluid–structure interactions (FSI), and their coupling to rigid-body dynamics.

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Code versioning system	git
Software code languages	C++
Legal code license	Apache License, Version 2.0
Computing platforms/Operating Systems	Linux, Mac OS, Microsoft Windows
Installation requirements & dependencies	Boost, Threading Building Blocks (TBB), SimBody
Link to developer documentation/manual	https://xiangyu-hu.github.io/SPHinXsys/
Support email for questions	c.zhang@tum.de, xiangyu.hu@tum.de

Software metadata

Current software version	0.2.0
Permanent link to executable of this version	https://github.com/Xiangyu-Hu/SPHinXsys
Permanent link to reproducible capsule	https://codeocean.com/capsule/6572430/tree/v1
Versioning system	git
Software code languages	C++
Legal software license	Apache License, Version 2.0
Computing platforms/Operating Systems	Linux, Mac OS, Microsoft Windows
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1. Introduction

Multi-physics problems are ubiquitous in natural phenomena and play key roles in a vast range of industrial applications. One typical example is the fluid–structure interaction (FSI) problem where flexible and deformable elastic structures are immersed in viscous fluids [1], and occurs in a broad variety of problems ranging from aerial animal flying and aquatic animal swimming to the flow of blood in the heart and throughout the cardiovascular system. Due to the inter-discipline characteristics and intrinsic complexities, computational modeling of multi-physics problems is highly challenging. An instance, taken from the human life systems, is the cardiac function which is composed of complex structures, i.e. four chambers (two atria and two ventricles), four valves (two semilunar valves and two atrioventricular valves) and blood vessels, and governed by the fully coupled electro-phyisological, mechanical and fluid dynamics [2]. Multi-physics modeling of cardiac processes, including the interaction of the cardiac electrophysiology system [3] with contractile muscle tissue [4], the sub-cellular activation–contraction mechanisms, as well as the hemodynamics within the heart chambers, has recently received tremendous attention and are recognized as the community's *next microscope, only better* [5]. However, an integrated model capable of simulating the fully coupled cardiac function is still in its infancy. As an open-source meshless, multi-physics and multi-resolution library, the long-term objective of SPHinXsys is an integrated computational framework for the further development of specialized simulators to investigate a large range of multi-physics, like cardiac function, problems.

2. Description

Smoothed particle hydrodynamics (SPH) [6–8] is a fully Lagrangian particle method, in which the continuum media is discretized into Lagrangian particles and the mechanics is approximated as the interaction between them with the help of a kernel, usually a Gaussian-like function. SPH is a meshless method, which does not require a mesh to define the neighboring interaction configuration of particles, however, the initial construction and updating the interaction configuration of particles are done according to the distance between particles. A remarkable feature of this method is that its computational algorithm involves a large number of common abstractions, i.e. particles, which brings the possibility of inherently linking to many physical systems. Therefore, SPH provides a substantial potential for modeling multi-physics problems. When the SPH method is used for studying multi-physics problems [9–11], the single-resolution approach can be rather expensive in applications where locally refined spatial–temporal resolution is required by a sub-system. For example, this is the case for FSI where the structure is relatively thin, i.e. the structure has a considerable small spatial scale compared to the fluid. As a consequence, a multi-resolution SPH method which is capable of employing various spatial–temporal resolutions for different sub-systems is desirable [11,10].

SPHinXsys presently (Version: 0.2.0) focuses on the unified continuum-mechanics modeling of fluid dynamics, solid mechanics, diffusion–reaction, and their coupling. The algorithms for the discretization of the fluid dynamics equations are based on a weakly compressible fluid formulation [12], which is suitable for the problems with incompressible flows, and compressible flows with low Mach numbers (less than 0.3). The solid dynamics equations are discretized by a total Lagrangian formulation [11,10], which is suitable to study the problems involving linear and non-linear elastic materials. The FSI coupling algorithm is implemented in a kinematic-force fashion, in which the solid structure surface describes the material-interface and, at the same time, experiences the surface forces imposed by the fluid pressure and friction.

SPHinXsys defines a collective objects and methods to be applied as libraries for a multi-physics and multi-resolution computation, being constructed and carried out in an application code. The core object and the core method are `SPHBody` and `ParticleDynamics`, respectively. While the former defines spatial and topological relations between particles, and the latter describes the corresponding physical dynamics of them. As shown in Fig. 1, the first stage is to create all the `SPHBodys` based on their realizations. There are `RealBodys` modeling fluid and solid bodies, and `FictitiousBodys` modeling observers which collect the computational data from `RealBodys` during the simulation. At the second stage, the topology of `SPHBodys` is constructed. The topology describes all the interacting `SPHBodys` for each individual `SPHBody`. After this, all `ParticleDynamics` will be defined. Specifically, each realization of `ParticleDynamics` corresponds all the discretized right-hand-side terms of a fluid or solid dynamics equation. If SPHinXsys is coupled with SimBody, one needs to create a `SimTK` system in which all `matters`, `mobility` and `forces` are defined. The SimBody-SPHinXsys coupling, as a realization of `ParticleDynamics`, includes computing forces on solid body for SimBody and imposing constraints of solid body by SimBody. Finally, `Output` is created to specify the data that will be saved in an external file during the computations.

3. Impact

SPHinXsys has shown its efficiency, accuracy and robustness for simulating fluid dynamics [10], solid mechanics and their coupling [11]. Here, three benchmark FSI tests, i.e., a hydrostatic water column on an elastic plate, a flow-induced vibration and a dam-break flow with elastic gate, are briefly summarized and readers are referred to Refs. [10,12,11] for more validations.

The first benchmark test studied here is the deformation of an elastic plate under hydrostatic pressure of a water column where an aluminum plate is suddenly exposed to it. According to Refs. [13,14], an equilibrium state reaches after initial oscillations and the equilibrium displacement at the plate mid-span can be obtained from an analytical model. Fig. 2(a) gives the time histories of the mid-span displacement, together with the convergence study with increasing spatial resolution of structure while the resolutions of fluid is constant. A high-order convergence of the middle-span displacement is observed. In the second benchmark, a two dimensional flow-induced vibration of a flexible beam attached to a rigid cylinder is studied. Fig. 2(b) shows the flow vorticity field and beam deformation at different time instants in a typical periodic movement when self-sustained oscillation is reached. Good agreements with previous computational result [15] are noted. Finally, we consider the deformation of an elastic plate subjected to a time-dependent water pressure, where free-surface flow is involved. The comparison between the numerical snapshots and the experiment presented by Antoci et al. [16] is illustrated in Fig. 2(c). It can be observed that the simulation results are in a good agreement with the experimental results.

Concerning the computational efficiency, with the multi-resolution treatments of SPHinXsys up to 240 and 960 times speed ups are achieved when the fluid–structure resolution ratio is 2 and 4, respectively. These computational efficiency analysis are carried out for the first benchmark.

4. Potential improvements

In the present version (Version: 0.2.0), SPHinXsys has accomplished its major solvers for typical multi-physics modeling. Meanwhile, a set of numerical studies for several bio-mechanical applications, e.g. venous valve and passive flapping of a fish-like body in flow, have been carried out to demonstrate the versatility and potential of SPHinXsys in simulating bio-mechanical systems.

In the future, one important aim is on developing an integrated total human heart simulator based on SPHinXsys. The heart simulator is expected to carry out numerical simulations of the total heart function [2] with high-resolution heart anatomy models and explore the possible

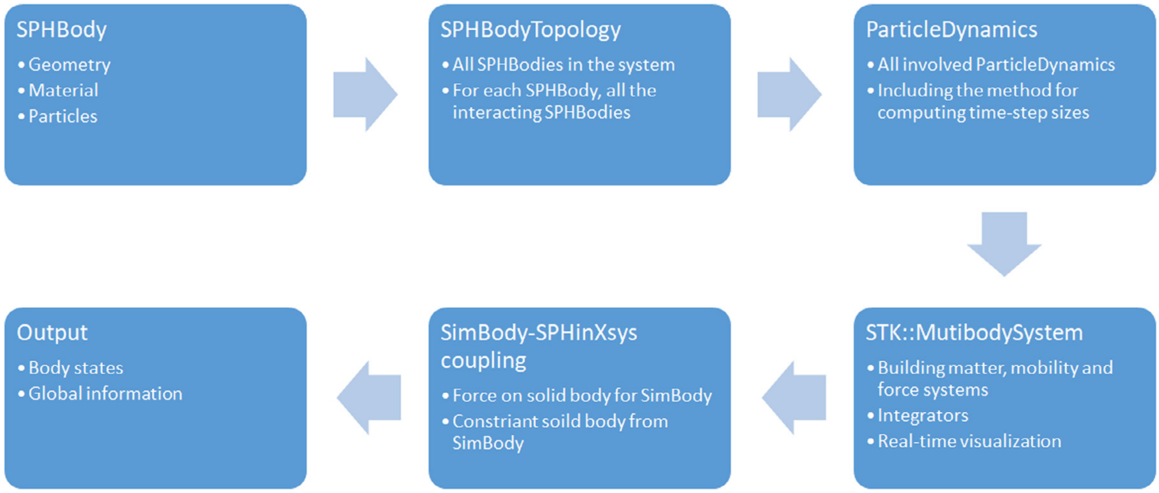
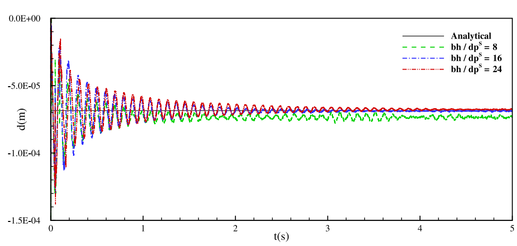
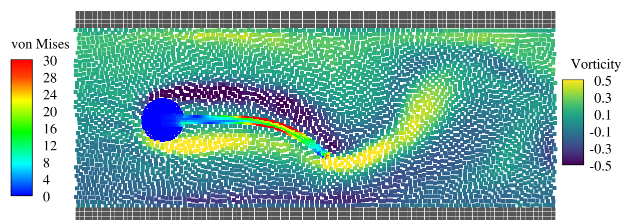


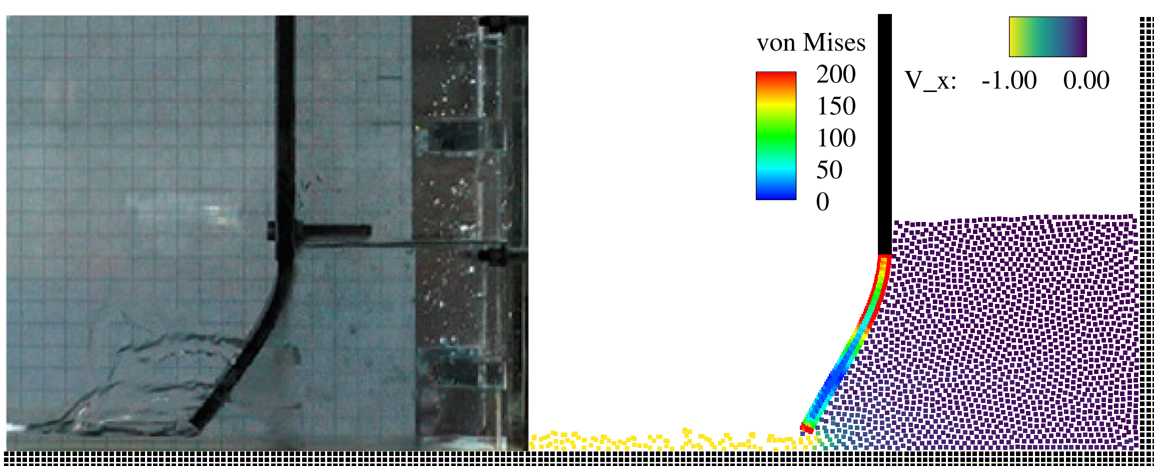
Fig. 1. Various steps of constructing a simulation using SPHinXsys.



(a) Plate under hydrostatic water



(b) Flow-induced vibration



(c) Dam-break flow through an elastic gate

Fig. 2. FSI benchmark validation for SPHinXsys with a fluid–structure resolution ratio of 2. (a) The time history of mid-span displacement of an elastic plate under a hydrostatic water column. (b) The flow vorticity field and beam deformation of flow-induced vibration of a beam attached to a cylinder. (c) Snapshots for dam-break flow through an elastic gate compared against experimental frames [16].

clinical applications. The integrative heart simulator allows us to model anatomically accurate heart in realistic physiological conditions. To this aim, models of the electrophysiology monodomain equation for Purkinje network and contractile muscular fibers, the myocardium mechanics, the valve dynamics and the complex haemodynamics will be developed and coupled. We expect that the multi-physics heart simulator will shed light on the complex interplay between the chemical, electrical and mechanical fields that are involved in the cardiac cycle and also complement and extend our understanding of cardiac diseases [5].

Another improvement would be optimizing the computational efficiency by implementing graphics processing unit (GPU) accelerators combined with many-core parallelization strategy.

CRediT authorship contribution statement

Chi Zhang: Writing - original manuscript, Writing - review & editing, Methodology, Software. **Massoud Rezavand:** Software, Writing - review & editing. **Yujie Zhu:** Software. **Yongchuan Yu:** Software. **Dong Wu:** Software. **Wenbin Zhang:** Software. **Shuoguo Zhang:** Software. **Jianhang Wang:** Methodology. **Xiangyu Hu:** Supervision, Writing - review & editing, Methodology, Software.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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