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SPHMPS 1.0: A Smoothed-Particle-Hydrodynamics Multi-Physics Solver

Iman Farahbakhsh [a,*], Benyamin Barani Nia [a], Erkan Oterkus [b]

[a] Department of Maritime Engineering, Amirkabir University of Technology, Tehran, Iran
[b] Department of Naval Architecture, Ocean, and Marine Engineering, University of Strathclyde, Glasgow, United Kingdom

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ABSTRACT

SPHMPS 1.0, developed within a Lagrangian framework, offers a robust solution for modeling multi-structure collision problems involving large plastic deformation and inherent thermal effects. Utilizing its innovative algorithm, SPHMPS 1.0 emerges as a versatile tool for researchers in the field of fluid-rigid-elastic structure interactions. By providing a comprehensive framework tailored to address these complex phenomena, SPHMPS 1.0 facilitates reproducible, extendable, and efficient research endeavors. Implemented in Fortran, its flexible algorithm ensures adaptability to a wide range of applications requiring solutions for fluid-rigid-elastic structure interaction problems.

Code metadata

Current code version	v1.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2024-39
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/4665023/tree/v1
Legal Code License	MIT License
Code versioning system used	git
Software code languages, tools, and services used	Fortran, CodeBlocks, Visual Studio Code
Compilation requirements, operating environments & dependencies	Fortran compiler
If available Link to developer documentation/manual	https://doi.org/10.1007/s42102-023-00110-y
Support email for questions	i.farahbakhsh@aut.ac.ir

1. Introduction

SPHMPS 1.0, a smoothed-particle-hydrodynamics multi-physics solver, stands at the challenging forefront of computational advancements in the field of structural collision. It employs the weakly compressible smoothed particle hydrodynamics method to address the complexities of large deformations engaged with thermal phenomena. Specifically designed to model multibody collisions involving structures undergoing substantial plastic deformation and temperature gradients, SPHMPS 1.0 represents a significant leap forward in our ability to simulate intricate physical phenomena.

In contrast to conventional monolithic Eulerian solvers [1–5], SPHMPS 1.0 as a Lagrangian solver, offering a unique and powerful framework for simulating the collision dynamics of both rigid and elastic structures. This Lagrangian approach proves to be especially advantageous in capturing thermal effects within the mushy zone of contact regions, making it a more viable and comprehensive solution. In this category of solvers one can address the SPHinXsys [6] that is a multi-resolution and multi-physics library and aims at modeling coupled multi-physics industrial dynamic systems.

This paper aims to delve into the algorithm of SPHMPS 1.0 and describe its impacts in the field of computational modeling of structural collisions, limitations, and future applications. The development repository of the code is accessible at https://github.com/imanfarahbakhsh/SPHMPS1.0.git and the permanent link to reproducible capsule is https://codeocean.com/capsule/4665023/tree/v1.

2. Software design and functionality

SPHMPS 1.0 is a specialized tool developed using FORTRAN, a high-level, general-purpose programming language that is particularly suited to numeric computation and scientific computing. The primary

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* Corresponding author.
E-mail addresses: i.farahbakhsh@aut.ac.ir (I. Farahbakhsh), benyaminbarani@aut.ac.ir (B. Barani Nia), erkan.oterkus@strath.ac.uk (E. Oterkus).

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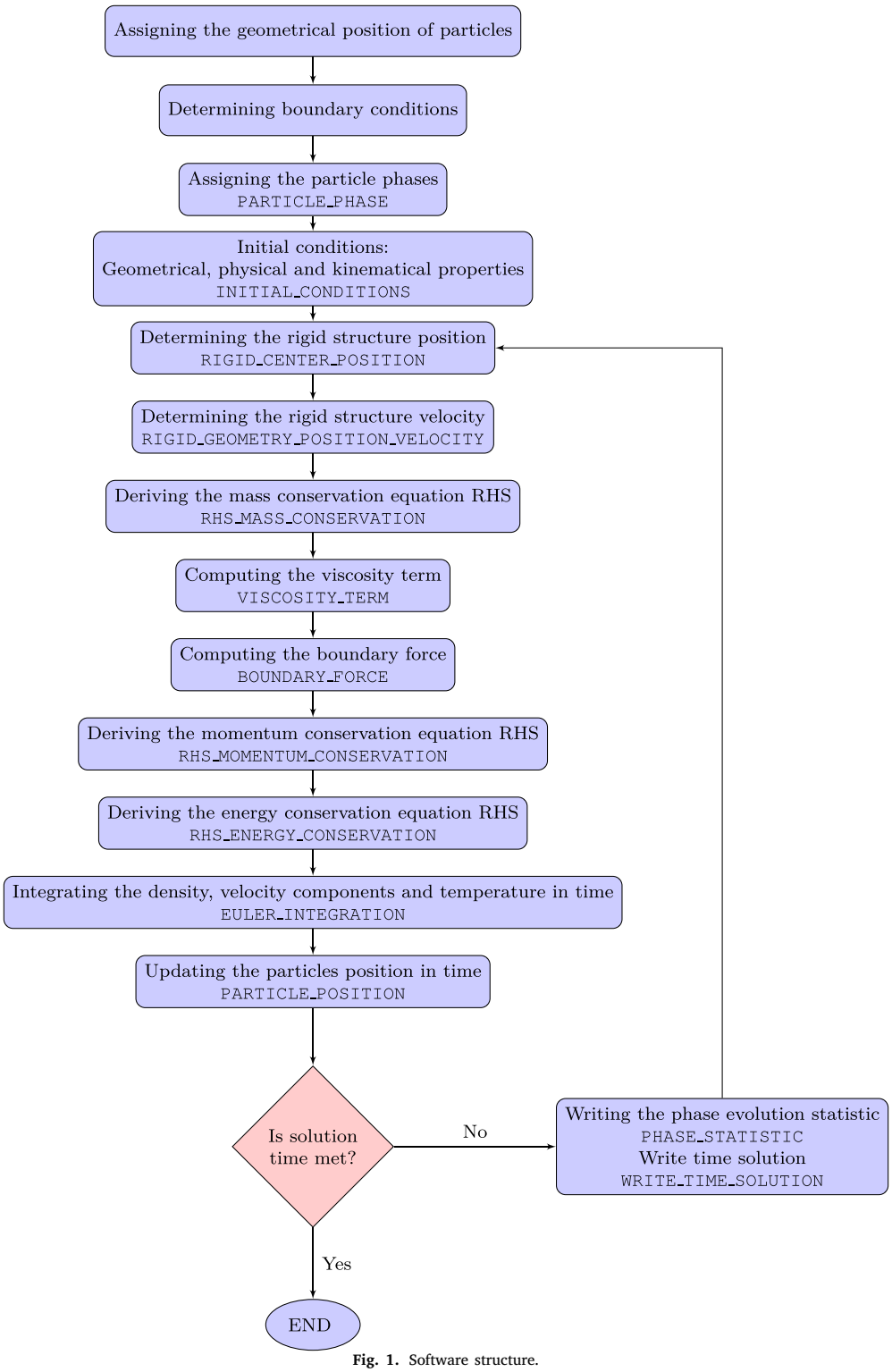

Fig. 1. Software structure.

function of this software is to solve the governing equations of multi-body interaction, particularly in scenarios where there are significant temperature gradients due to collision and plastic deformations. The software employs a weakly compressible smoothed particle hydrodynamics (WCSPH) method to solve these governing equations. WCSPH is a computational method used for simulating the mechanics of continuum media in Lagrangian framework, and is particularly effective in scenarios involving complex boundary conditions and large deformations. The software is modular in design, consisting of one main module and 21 subroutines. This modular structure allows for efficient code management and potential scalability, as each subroutine can be developed, tested, and debugged independently. It also enhances the readability and maintainability of the software, making it easier for other developers to understand and contribute to the project. In summary, this FORTRAN-based software is a powerful tool for solving complex multibody interactions under significant temperature gradients, leveraging the WCSPH method for accurate and efficient computations. Its modular design ensures its maintainability and scalability, making it a robust and reliable tool for scientific computing. The whole software structure is presented in Fig. 1.

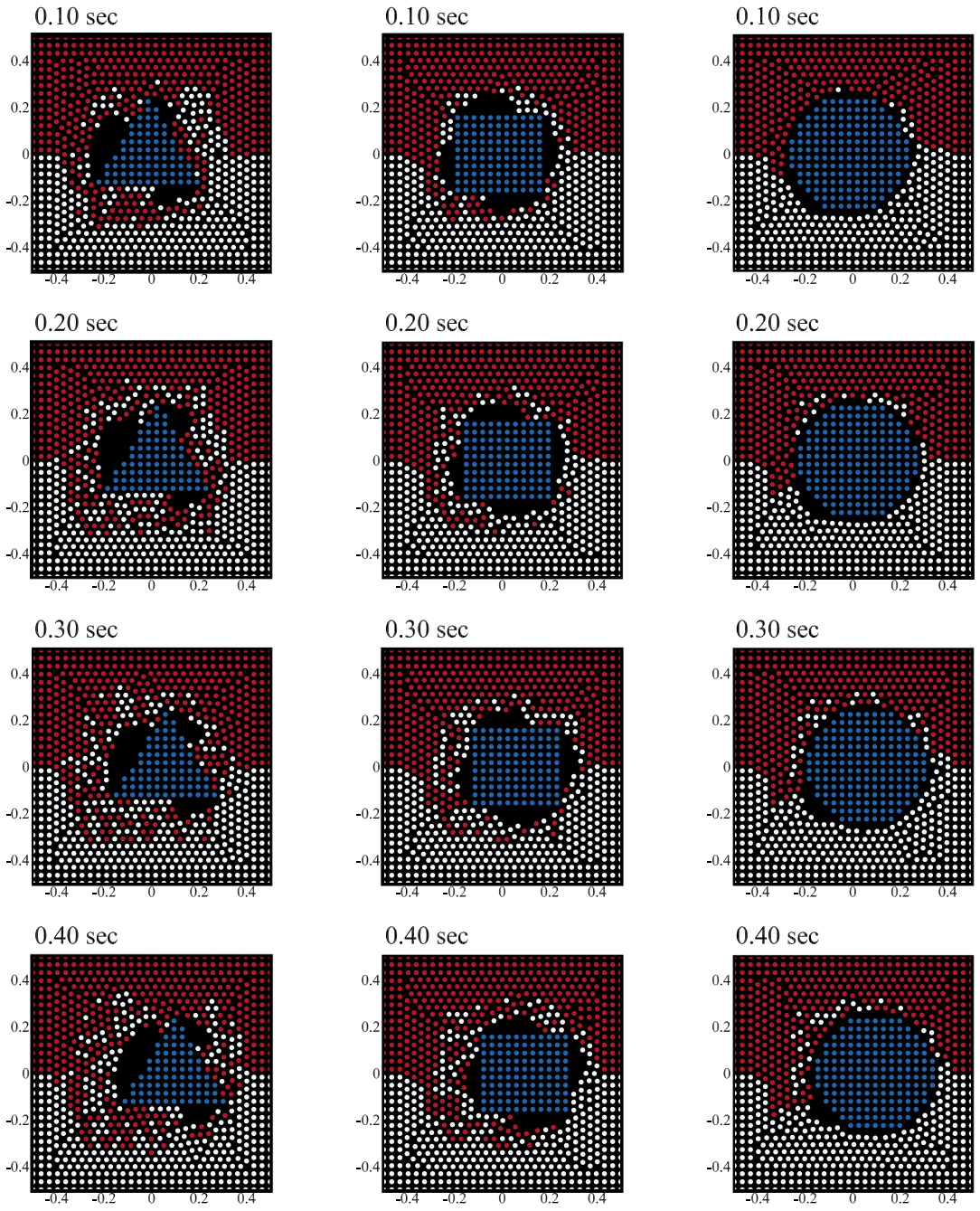

Fig. 2. Particles migration patterns after every two complete rotations of triangular, square and circular pins.

The main structure of the software is constituted from several subroutines, each with specific functions. The initial subroutines are devoted to assigning the geometrical position of all particles and setting up the boundary conditions. The subroutine `PARTICLE_PHASE` is developed for determining the particle types and characterizing the particles from a material point of view. The subroutine `INITIAL_CONDITIONS` is devoted to assigning the initial conditions for the physical and kinematical properties of the characterized particles. If there is any rigid structure in the problem, the subroutines `RIGID_CENTER_POSITION` and `RIGID_GEOMETRY_POSITION_VELOCITY` compute the rigid center position and velocity in each time step, respectively. The subroutines `RHS_MASS_CONSERVATION`, `RHS_MOMENTUM_CONSERVATION`, and `RHS_ENERGY_CONSERVATION` are developed for computing the right-hand side of the mass conservation equation, momentum conservation equations, and energy equation, respectively. The density, velocity components, and temperature are integrated in time using `EULER_INTEGRATION`. The auxiliary subroutines `VISCOSITY_TERM` and `BOUNDARY_FORCE` are designed for computing the viscosity effect in the mushy zone due to large plastic deformation and the boundary force due to interactions with rigid particles, respectively. The subroutine `PARTICLE_POSITION` updates the particle positions in time. The subroutines `PHASE_STATISTIC` and `WRITE_TIME_SOLUTION` are designed for writing the results such as particle's positions, density, velocity components, temperature, and can present a locus of particles.

In summary, the software is structured in a way that allows for efficient computation and data management, with each subroutine performing a specific task in the overall process. This modular approach enhances the software's flexibility and adaptability, making it a robust tool for solving complex multibody interactions.

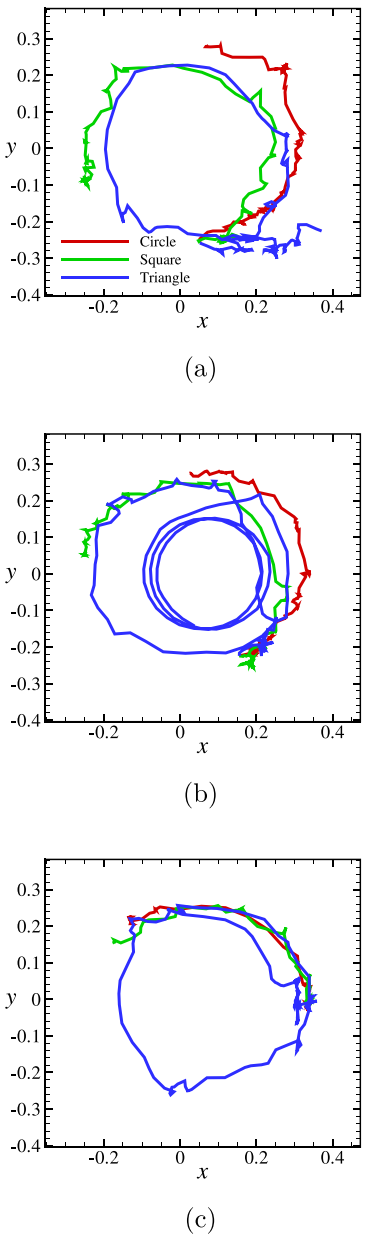

Fig. 3. The traces of three migrated particles with starting positions (a) (0.051,−0.258), (b) (0.155,−0.224), and (c) (0.327,−0.017) under the effect of translational and rotational motions of circular, square and triangular pins in FSW process [7].

3. Impact overview

SPHMPS 1.0, leveraging the weakly compressible smoothed particle hydrodynamics (WCSPH) method, represents a notable stride in computational modeling applicable to diverse scenarios. Its application in simulating material flow during friction stir welding (FSW), considering various pin geometries, is just one facet of its broader utility [7]. By solving governing equations of mass, momentum, and energy conservation, the software offers a comprehensive understanding of the fundamental physics involved in material mixing processes. A sample of results extracted from SPHMPS 1.0 is shown in Fig. 2 and illustrates the mixing process of particles in the mushy zone around various configurations of pins in FSW. The validation of simulation results through agreement with experimental evidence enhances the software's reliability, establishing it as a versatile tool for researchers and practitioners across diverse fields. SPHMPS 1.0 employs a binary supervised machine learning model for classifying and tracking particle phases, distinguishing it from similar software like SPHinXsys [6]. The results of postprocessing with this model are presented in Fig. 3, which includes the traces of three particles initiating their migration between two phases under the effects of rotational and translational motion from three different pins [7].

The statistical study conducted with the software extends beyond the simulation of material flow during FSW, providing insights into the complex mechanism of particle migration between two or more colliding structures. Through particle tracking and spatio-temporal distribution analysis, the software facilitates a nuanced examination of how different pin shapes influence particle relocation, serving as a valuable tool for optimizing processes beyond welding.

The software's versatility lays the groundwork for future applications, ranging from destructive collisions and high-speed deformations to failure analysis, crack propagation, and structure-structure interaction with large deformation and thermal effects. This adaptability positions the software as a valuable asset with implications across a spectrum of domains where material dynamics play a crucial role.

4. Limitations

Despite the promising capabilities of the developed software in simulating the material flow in friction stir welding (FSW) with various pin geometries, several limitations exist in the current version of the software, which warrant consideration for future enhancements.

Two-Dimensional Scope: The current version of the software is specifically tailored for two-dimensional problem settings. While this allows for insightful investigations into the initial moment interactions of pins with workpiece materials, the restriction to two dimensions may limit the applicability of the software in scenarios where three-dimensional effects play a crucial role. Future developments could focus on extending the software to handle three-dimensional simulations, providing a more comprehensive representation of real-world welding processes.

Simplified Viscosity Model: In its current state, the software employs a general fluid model for incorporating viscosity effects, which serves the purpose but may lack the sophistication needed for more nuanced simulations. Recognizing this, future versions of the solver could benefit from the inclusion of additional viscosity models, allowing users to choose from a range of options based on the specific characteristics of the materials involved. This enhancement would contribute to a more accurate representation of non-Newtonian behavior in the simulated mushy zone around the pins.

Constant Thermal Properties: The thermal properties, including heat conduction coefficient, film coefficient, and specific heat, are treated as constants in the current version of the solver. While this simplification facilitates computational efficiency, it may not capture the full complexity of real-world scenarios. A more realistic representation could involve considering these thermal properties as variables, allowing for dynamic changes during the simulation. Future iterations of the software could explore this avenue, enabling a more detailed analysis of the thermal aspects of the friction stir welding process.

Addressing these limitations in subsequent versions of the software will not only enhance its versatility but also improve its fidelity in simulating the intricate dynamics of material flow during friction stir welding, making it an even more valuable tool for researchers and practitioners in the field.

5. Future applications

The developed software, leveraging the weakly compressible smoothed particle hydrodynamics (WCSPH) method, exhibits significant potential for a broader array of applications beyond its current focus on modeling material flow in friction stir welding (FSW) with different pin geometries. The unique capabilities of the software, as

evidenced by its success in simulating the initial moments of pin and workpiece interactions, pave the way for future applications in diverse domains.

Modeling Destructive Collisions: The software's adaptability and robust numerical framework position it as a promising tool for modeling Destructive collisions. Whether in industrial settings or research scenarios, where understanding the dynamics of collisions is crucial, the software could be employed to simulate and analyze the intricate material interactions during such events.

High-Speed Deformations: The inherent ability of the software to capture the nuances of material flow in dynamic processes makes it well-suited for simulating high-speed deformations. This could find application in scenarios involving rapid structural changes, such as impact events or high-velocity material transformations.

Failure Due to Collision: With a focus on particle migration and material mixing, the software can be extended to study failure mechanisms resulting from collisions. This includes investigating how the distribution of particles influences structural integrity and identifying critical points where failure is likely to occur.

Crack Propagation: The software's capability to model material flow and interactions makes it an ideal candidate for studying crack propagation. By incorporating fracture mechanics principles, future versions of the software could contribute to understanding how cracks propagate through materials under different conditions.

Structure-Structure Interaction with Large Deformation and Thermal Effect: The software's applicability extends to scenarios involving complex structure-structure interactions characterized by large deformations and thermal effects. This could include simulations of thermal-structural coupling in various engineering applications, offering insights into the coupled behavior of materials.

Material Flow in Multi-Structure Interactions: The software's ability to handle material flow in the interaction of two or multiple structures positions it as a valuable tool for a wide range of applications where understanding the intricate dynamics of material interactions is paramount. This includes scenarios in manufacturing, materials science, and other fields where multi-structure interactions play a crucial role.

As the software evolves, enhancements in its numerical methods and computational efficiency will likely broaden its scope for these future applications, providing a versatile and powerful tool for researchers and engineers across diverse disciplines. These potential applications underscore the software's significance in advancing simulation capabilities for complex physical phenomena.

CRediT authorship contribution statement

Iman Farahbakhsh: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Benyamin Barani Nia:** Writing – review & editing, Visualization, Resources. **Erkan Oterkus:** Writing – review & editing.

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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