Abstract of the dissertation titled

**Application of a novel meshfree modeling algorithm to hydraulic engineering problems**

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Introduction, motivation

The numerical methods providing the approximate solution of partial differential equations can be classified from different points of view. One of them is the procedure of discretization of the continuum system. Although the idea of particle-based modeling is as old as that of the mesh-based modeling, the latter dominated the area of numerical analysis for almost half a century. It was not earlier than the 1990s when significant advances were made in particle-based modeling, yet they managed to prove their reason for existence in numerous areas of scientific computing. One can consider discrete element methods as well as collocation schemes as particle-based meshfree methods. The most widespread and fundamental particle-based method today is the smoothed particle hydrodynamics (SPH), which has been applied in many areas of fluid flow modeling successfully in the past three decades.

Due to their attractive properties, particle-based numerical methods enjoy increasing attention in many fields of engineering applications. In contrast with mesh-based methods like the finite element method (FEM), particle-schemes have more flexible and adaptable spatial discretization of the computational domain of any shape, especially in case of large deformations involving topology changes even with domain-splitting.

Most of the characteristic features of particle-based numerical schemes are fundamentally different from that of mesh-based methods. Some of these differences are the lack of internodal structure (mesh), the persistent changing of nodal connectivity, and the overlapping spatial covering of the computational domain. Relying on such differences, most of the advances related to particle methods show that being robust in different circumstances makes meshless schemes complementary rather than competing with mesh-based methods, and vice versa.

In the area of both scientific computing and industrial applications, the utilization of the recent developments of meshfree methods suffers from severe difficulties. The currently available open-source packages usually do not provide sufficient flexibility in terms of either the applied numerical methods or the mathematical models. Since the numerical methods themselves are changing rapidly, the application of the most recent theories is potentially obstructed by the decisions of the software developers. Therefore the implementation of rather specialized simulation tools is inevitable.

In the case of mesh-based modeling, the complete separation of the numerical methods from the mathematical models has been proven to be an efficient approach in general-purpose computing. The available generic algorithms (e.g. FEniCS and Deal II) provide highly flexible usage in contrast with the conventional tools. Although these tools have been successfully applied in several scientific and even industrial
areas, the same approach in meshfree modeling has been appeared only during the recent years.

In my dissertation I introduce the design and implementation of a general-purpose meshfree modeling algorithm relying on a novel approach in this area. Then I use the algorithm to model and investigate different dynamical systems.

**Objectives**

During my research I aimed to design and implement a general-purpose simulation tool that facilitates the development and application of meshfree numerical methods in the area of scientific computations. I formulated the following requirements and objectives in terms of the capabilities of the algorithm:

- the complete separation of numerical methods from the mathematical models,
- three-level abstraction that allows the definition of free-form equations without programming tasks (bottom level: low-level algorithms, intermediate level: definition of interaction laws, high-level: definition of the mathematical models)
- the implementation of the numerical methods without the deeper knowledge of the solver core.

The objectives concerning the application of the simulation tool I formulated the following goals:

- implementation of a suitable meshless numerical method, the smoothed particle hydrodynamics (SPH),
- verification of the algorithm and the SPH implementation through simple hydraulic test cases,
- investigation of different hydrodynamic models by means of the implemented solver, solution of the shallow water equations, modeling large scale circulations in shallow lakes induced by spatially and temporally constant wind shear stresses,
- development of the spatially adaptive variant of SPH using the general purpose simulation tool.

**The applied numerical method**

Fulfilling the objectives, I implemented the algorithm in C++, which provides effective tools and sufficient freedom for the three-level abstraction.

Although during the development of the algorithm, the main goal was the generality, requiring both the free-form definition and configuration of the mathematical models and the flexible choice of the numerical methods to be applied, in the present work I focused on the widespread smoothed particle hydrodynamics method.
The conventional SPH is a purely meshfree, explicit, Lagrangian collocation technique, allowing the approximation of partial differential equations in such a way that through a suitable discretization it subdivides the continuum field to a set of interacting elementary material points governed by a system of ordinary differential equations, which can be solved significantly simpler using numerical integration. The hydrodynamic aspects of the method are remarkable: according to its Lagrangian nature, it can be efficiently used for highly complex transient flows dominated by inertial forces with the presence of free surfaces, where mesh-based methods often suffer from serious bottlenecks.

Using the SPH method, I modelled weakly compressible two- and three-dimensional fluid flows by the approximate solution of the Navier-Stokes equations using the SPH method, and investigated the wind induced circulation in shallow lakes solving the shallow water equations numerically. By means of the simple reconfiguration of the solver, I built a mathematical model governing the dynamics of spatially coupled phase oscillators, and applied for the investigation of diluted systems.

**Principal results**

Recently, a notable need appeared for highly flexible numerical meshfree simulation tools, which allow the efficient definition of mathematical models. I started the development of the algorithm motivated by the similar tools of finite element methods. The results are summarized in the subsequent sections.

**Design of the algorithm for meshfree methods**

Despite the fact that the flexible general-purpose computing approach has appeared for mesh-based methods and successfully applied in several areas of scientific and engineering applications, the same approach started to evolve only during the recent years.

**Principal result 1.**

*Havasi-Tóth, B. (2019a), Tóth, B. Szabó, K. G. (2014)*

Utilizing the similarities among meshfree Lagrangian numerical techniques, I have defined a general formulation of ordinary differential equations describing the dynamics of interacting material points. By defining arbitrary functions over a spatially distributed material point set, the general formulation potentially covers both a wide range of meshfree collocation schemes and models of genuinely discrete phases as well by considering them as combinations of nodal interaction laws.
One of the most important aspects of the algorithm is that it considers the particle-based numerical methods as a combination of functions describing pairwise interactions, therefore after the definition of suitable interaction laws as mathematical functions, almost arbitrary system of ordinary differential equations can be constructed and solved. A notable consequence of this approach is that these equations are compatible with the mathematical models both genuinely discrete systems (discrete element method or molecular dynamics) as well as the discretized equations of continuum problems (through collocation techniques). Therefore, the particle methods can be considered as simple operator nodes in the class hierarchy of expressions used for parsing free-form user-defined equations and expressions. Hereby, the hierarchy can be simply extended by arbitrary interaction laws, hence particle methods.

![Diagram of the class hierarchy of the expression parser of the algorithm. The nodes in the lowest row represent the numerical methods that are the interaction laws.](image)

**Figure 1: the class hierarchy of the expression parser of the algorithm. The nodes in the lowest row represent the numerical methods that are the interaction laws.**

**Reduction of numerical resolution with exact conservation of angular momentum**

The local changing of numerical resolution is frequently required during the numerical solution of partial differential equations. Among a few other reasons, it is usually the case that in order for the numerical error to be approximately constant throughout the computational domain, the resolution has to be finer in the vicinity of large gradients of the solution. Besides that, mostly in fluid flow modeling, the solution is of interest only over a limited portion of the geometry, while the rest of the domain (which is often referred to as the far-field) is built only to keep the boundary conditions sufficiently far away from the specific zone. While in the case of mesh based finite volume methods, the theories behind the spatially variable resolution are based on
well-known and robust considerations, in case of SPH, the Lagrangian frame makes the problem less straightforward. Merely changing the particle sizes is not satisfactory, since the particles follow material trajectories, hence they simply drift away from the area of interest, making coarser particles formerly placed in the far-field occupy the same locations. Therefore currently, the widely used techniques dynamically remove and introduce particles of the desired size by splitting and coalescing over prescribed locations. The process of splitting and coalescing can be performed by the minimization of a suitably chosen numerical error. However, former techniques introduce significant error in the computation due to the pairwise coalescing, which results in a single particle lacking the minimal degree of freedom to inherit the angular

![Diagram](image)

**Figure 2:** results of the two-dimensional Taylor-Green vortex pattern with different resolutions. Particles are colored by their instantaneous velocity magnitudes. From left to right: coarse resolution, fine resolution and coarse resolution with local refinement.

![Diagram](image)

**Figure 3:** kinetic energy dissipation corresponding to the different resolution cases compared to the analytical solution.
momentum of the configuration before merging. Circumventing this issue, I proposed an improvement of the coalescing techniques according to the followings.

Principal result 2. 
(Havasi-Tóth, B. (2019b))
I have elaborated a correction of the existing varying resolution SPH particle coalescing schemes that exactly preserves the local angular momentum. I have shown that

2.1. the loss of angular momentum due to the coalescing of particle pairs can be eliminated by involving particle triplets in the original configuration.

2.2. in case of merging the particle triplets to pairs, the smoothing radii of the new particles can be computed iteratively using the smoothing kernel function values obtained from the density scatter formulation,

2.3. by setting the spatial separation parameter $\eta$ to 0.9, the proposed technique results in a sufficiently uniform particle distribution in the coarsed configuration.

Modeling free surface solitary wave with SPH
Following the implementation of the algorithm, by the definition of the appropriate interaction classes of the SPH interaction laws, the solver became capable to model the dynamics of material points, more specifically even to investigate fluid dynamic problems. I verified the solver through mostly known test cases.

![Figure 4: evolution of solitary wave propagation speeds in the 10 m long channel. The table shows the evolution of the waves traveling along the channel with small (a., c., e.) and the large (b.,d.,f.) amplitudes. The dx values in the table show the particle sizes](image-url)
I performed computations of free surface solitary waves traveling along a straight channel to determine the wave shape and propagation speeds. I compared the results of the weakly compressible model to measurement data and first and second-order theories.

**Figure 5:** the SPH solitary wave shapes corresponding to the simulation cases shown in the table at $t=6$ s (solid lines), and the analytical solution of the KdV equation (dashed lines).

**Modeling wind induced circulation in shallow lakes**

In the case of fluid flow problems of engineering applications, the extension of the flow field often varies strongly in different the directions, hence its size in one or two directions is orders of magnitudes smaller or larger than the others. Flows in shallow water bodies such as lakes have such properties. The complete three dimensional description of these types of flows is expensive, but usually also unnecessary. By assuming that the vertical flow conditions in shallow lakes are not significant in terms

**Figure 6:** circulation in the elliptic lake. Left: Curto et al. 2006, right: SWE-SPH including the wind shear stress. The white arrow shows the constant wind direction.
of large scale circulation, we can perform the depth averaging of the flow field to obtain the so-called shallow water equations, which can be solved much easier. The large scale circulation in shallow lakes are induced by the wind shear stress over the surface of the water. However, in order to induce depth averaged flow in the lake, either the wind shear stress distribution or the bathymetry of the lake has to be a function of space. The latter introduces vorticity in the flow field through the gradient field of the bathymetry.

I built the SPH model consisting of the shallow water equations (SWE-SPH) in the solver and extended the equations with the wind shear stress term, then I applied the model to shallow lakes with simple geometries.

The result of the computations regarding both the solitary waves in the straight channel and wind induced circulations in shallow lakes have been summarized as follows.

### Principal result 3.

*(Tóth, B. (2017), Tóth, B. (2018))*

I have shown the followings:

1. by increasing the numerical resolution, the SPH results converge to the theoretical second-order approximation,
2. the propagating and diffusing SPH solitary waves march through a series of stationary solitary wave solutions,
3. the SPH solitary wave shapes are in a good agreement with the KdV solutions as well as the measured wave shapes.

Then, by the reconfiguration of the mathematical model passed to the solver, I modelled the wind induced circulating flow in shallow lakes with simplified geometries.

4. I have extended the SPH discretization of the shallow water equations with the constant wind shear force. I showed that the SPH method is suitable for the qualitative description of wind induced flows in shallow lakes: the model predicts the water surface inclination accurately, but underestimates the depth averaged flow velocities.

### Modeling the dynamics of spatially coupled phase oscillators

After the verification of the solver, I investigated the synchronization of spatially coupled phase oscillators using the Kuramoto model.

Synchronization is a collective behavior observed in many fields. It is a result of the interaction between oscillators capable of adjusting their rhythms/natural frequencies. To model synchronization of coupled phase oscillators the Kuramoto model proposed in 1975 is often used, for example, to investigate the collective behavior of lasers, neurons and social groups. One of the famous application of the Kuramoto model is the modeling of the synchronization of the periodic flashing of fireflies (*Pteroptyx malaccae*). This model was also used to describe the interesting phenomena related to,
a species of firefly capable of synchronous firing with almost no phase lag. This can be attributed to this insect's ability to alter its flashing frequency in response to external stimulus. Taking the inertia of the phase into account, the Kuramoto model can produce hysteretic behavior. For instance, in the case of the insects it can be observed that despite the requirement of certain lighting conditions for the spontaneous synchronization to be occured, the synchronous state may remain stable while changing the lighting even if the system would never reach that state with asynchronous initial conditions.

According to the simplest model, all the oscillators are coupled identically with all the others, however, in the reality it is rarely true. Therefore, the coupling of phase oscillators are usually diluted in most numerical computations.

In the course of my work, oscillators with phase inertia have been modelled, while the coupling strengths were considered to be the function of the euclidian distance between the spatially distributed oscillators. The distance dependent strengths have been determined using zeroth- and first-order smoothing kernel functions. The dynamics of the system have been investigated with various initial conditions and different rates of dilutions.

Principal result 4.
(Fehér, E., Havasi-Tóth, B., Kalmár-Nagy T. (2020))

I have investigated the dynamics of diluted spatially coupled phase oscillators. Using zeroth and first order kernel functions for the determination of pairwise coupling strengths, different cases have been investigated in terms of the influence radii, the number of oscillators and the spacing between the oscillators. I have shown that

4.1. due to the dilution based on the spatial kernel functions, local synchronization groups have been formed in various ranges depending on the coupling strength value \( K \),

4.2. increasing the coupling strength, the local groups have been broken in such a way that both the global and local synchronization suffered from a temporary but significant drop before the globally synchronized state occurs,

4.3. within the investigated range, the qualitative behavior of the synchronization dynamics depends merely on the value of the relative kernel radius \( q \).
Figure 7: states of the system of spatially coupled oscillators depending on the coupling parameter K. The relative kernel radius is $q=0.46$, $\Delta = 0.6$, $\Delta x = 0.05$, $N = 400$ applying first order kernel-function. a) Time series of the order parameter $R$ for different values of $K$ calculated for IC1. For $K_{C1} < K < K_{C2}$, $R$ has an oscillatory nature. b) Final phases of the oscillators in polar form at $t=500s$ illustrating the different states of the system calculated for IC1. c) States of the system and the time average $\bar{R}$ of the order parameter depending on the coupling parameter $K$. IC1 and IC2 represent asynchronous and synchronous initial conditions.
Figure 8: synchronization in case of different number of oscillators, various influence radii, initial conditions and grid sizes. Top: $q=\text{constant}$. Bottom: $\Delta=\text{constant}$. It can be seen that the dynamics of the system is governed by the relative influence radius $q$. 
Publications connected to the principal results

Journal papers (in english)

Journal paper (in hungarian)

Conference paper (in english)