

# Towards oscillation-free spectral ISPH scheme with high-order wall boundary conditions

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## I. INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) method is considered to be an alternative for traditional mesh-based method in the area of computational fluid dynamics (CFD). The Lagrangian feature of SPH makes it attractive for specific types of highly nonlinear applications such as multi-phase flow [1]. However, compared with the mature mesh-based methods which have well-established high order convergence theory, there are still a range of grand challenges that need to be thoroughly investigated [2]. To better understand and contribute to the remaining challenges in convergence and efficiency, this paper presents a novel spectral SPH scheme by building upon the convolution theorem. In a similar manner to mesh-based methods, a Fourier basis function is only applicable to periodic boundary conditions which limits the applications for spectral methods in complex flows. Previous research on implementing Discrete Trigonometric Transform (DTT) into spectral method have demonstrated success. Wise et al. [3] proposed a pseudospectral time domain (PSTD) method that a family of spectral collocation methods based on the use of a sine or cosine basis were described for discretising the wave equation. Apart from application in fluid mechanics, Paus et al. [4] applied the DST/DCT-based solvers to the elasticity of heterogeneous materials.

In light of the above, DTT is applied in this work for calculating the symmetric convolution. Furthermore, to extend the solver's capability for simulating wall boundary condition with Cartesian particle arrangement, the combination of the scheme with the Radial basis function based Immersed Boundary Method (RBF-IBM) is also investigated. To the best of the authors' knowledge, this is the first time that the discrete trigonometric basis function is used for convolution in SPH.

In the following sections the IBM-DTT-ISPH scheme is presented, followed by the convergence study through a 2D field function. The performance of the full solver is validated by classical CFD test case before a possible path of the future development.

## II. MATERIAL AND METHODS

### A. Governing equations and Time integration

The incompressible Navier-Stokes equations are given in Eulerian form as:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{f}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

where  $\mathbf{u} = [u, v, w]$  is the velocity in three dimensions,  $\rho$  is density,  $p$  is pressure,  $\nu$  is the kinematic viscosity and  $\mathbf{f}$  is body force (e.g. IBM force, gravity). The first-order projection method [5] is one of the most popular approaches for integrating (1) and (2) by projecting an intermediate velocity  $\mathbf{u}^*$  onto a divergence-free space. Pressure is obtained by solving the pressure Poisson Equation (PPE) and thus the incompressibility is enforced. Given that the first-order projection method has only first-order of accuracy in time which could hinder the overall accuracy results of the full solver, a third-order Runge-Kutta (RK3) is used to ensure the temporal error does not contaminate the spatial solution. The main steps are:

1) Calculate an intermediate velocity  $\mathbf{u}^*$  from the advection and viscous term with sub-step  $k$  and sub-step  $k-1$ :

$$\mathbf{u}^* = \mathbf{u}^k - \Delta t (g_k \mathbf{F}^k + z_k \mathbf{F}^{(k-1)} - a_k \nabla \tilde{p}^k + a_k^{(k+1)}), \quad (3)$$

with

$$\mathbf{F}^k = \mathbf{u}^k \cdot \nabla \mathbf{u}^k + \nu \nabla^2 \mathbf{u}^k. \quad (4)$$

and  $\tilde{p}^k = \frac{1}{a_k \Delta t} \int_{t_k}^{t_{k+1}} p dt$  and  $\tilde{f}^k = \frac{1}{a_k \Delta t} \int_{t_k}^{t_{k+1}} f dt$  is the time average pressure and body force within each sub-step  $k$ .

2) Calculate the divergence of the intermediate velocity  $\mathbf{u}^*$  and solve the PPE to obtain the pressure increment  $\phi$ :

$$\nabla^2 \phi = \frac{\rho}{\Delta t} a_k \nabla \cdot \mathbf{u}^*. \quad (5)$$

Here  $\phi$  is the pressure incremental within each sub-step.

3) Calculate the velocity for the next sub-step  $\mathbf{u}^{k+1}$ :

$$\mathbf{u}^{k+1} = \mathbf{u}^* - a_k \frac{\Delta t}{\rho} \nabla \phi. \quad (6)$$

and the pressure should be added by  $\Delta \phi$  until one physical time step finishes.

### B. Spectral approximation of differential operators

For the traditional physical space SPH operators, the integral representation of the gradient of a field function reads :

$$\nabla f(x) = \int f(x') \nabla W(x - x') dx', \quad (7)$$

comparing (7) with the definition of the convolution of two functions  $f$  and  $g$ ,

$$f * g = \int f(\tau) g(t - \tau) d\tau. \quad (8)$$

It can be found that (7) and (8) share the same form, which is also the original mathematical formulation of the SPH approximation. Replacing the  $g$  by the first derivative of the kernel function gives the spectral SPH equivalence of the function's gradient:

$$\nabla f = f * \nabla W. \quad (9)$$

Then, it is naturally convenient to take the advantage of the convolution theorem :

$$f * g = (\mathcal{F})^{-1}(\mathcal{F}(f) \cdot \mathcal{F}(g)). \quad (10)$$

Here the symbol  $\mathcal{F}$  indicates the Fourier transform such as:

$$\mathcal{F}(f(x)) = \hat{f}(\xi) = \int f(x) e^{-i2\pi\xi x} dx. \quad (11)$$

Substituting (10) into (9) leads to the formulation of the spectral SPH gradient:

$$\nabla f = \mathcal{F}^{-1}(\mathcal{F}(f) \cdot \mathcal{F}(\nabla W)). \quad (12)$$

From the spectral formulation, it is found that the convolution in the physical space is converted to the element-wise multiplication in the spectral space. Meanwhile, the Fast Fourier Transform (FFT) algorithm further reduces the arithmetic complexity from  $O(N^2)$  to  $O(N \log N)$ .

Since the Fourier transform is limited to periodic boundary conditions, to extend the capability of the spectral SPH scheme, we replace the Fourier basis function by a group of trigonometric basis functions. Taking the 2D Dirichlet boundary condition as an example, for a collocated particles distribution, this corresponds to the first type discrete sine transform (DST-I) which is,

$$\hat{f}_k = 2 \sum_{j=0}^{n-1} f_j \sin \frac{\pi(j+1)(k+1)}{n+1}. \quad (13)$$

Similarly, the first type discrete cosine transform (DCT-I) from (14) is implemented to satisfy Neumann boundary conditions.

$$\hat{f}_k = 2 \sum_{j=1}^{n-2} f_j \cos \frac{\pi j k}{n-1} + \hat{f}_0 + (-1)^k \hat{f}_{n-1}. \quad (14)$$

It is important to note that for all the DTT-based spectral SPH methods, due to the symmetric/antisymmetric properties of the kernel derivatives, only half of kernel derivatives (1D) and a quarter of kernel derivatives (2D) are needed for the discretization.

### C. Radial Basis Function (RBF) based Immersed Boundary Method (IBM)

Following [6], the IBM force is defined differently as

$$\mathbf{f}^{n+1} = \epsilon \left( -\nu \nabla^2 \mathbf{u}^n + (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n + \frac{1}{\rho} \nabla P^n + \frac{\mathbf{u}_{IB}^{n+1} - \mathbf{u}^n}{\Delta t} \right), \quad (15)$$

where  $\mathbf{u}_{IB}$  is the velocity inside the immersed boundary and parameter  $\epsilon$  is a scalar field acting as a mask which equals to 1 inside the immersed boundary and 0 everywhere else. This scalar field reduces the PPE to a Laplacian equation inside the immersed boundary.

The next step is to define  $\mathbf{u}_{IB}$  so that the no-slip boundary condition on the immersed boundary can be satisfied. One simple way is to directly use zero velocity inside the body (referred to IBM-simple scheme). This introduces a discontinuity across the boundary which will lead to Gibbs-like phenomenon in the flow properties. To avoid this, we use the Radial Basis Function (RBF) extrapolation as it is automatically multi-dimensional and it is consistent with the SPH kernel's radius support. To begin, the value of a function  $\mathbf{u}_{IB}$  at the unknown points  $\mathbf{x}$  can be obtained from the interpolation points  $\mathbf{x}_i$  by :

$$u_{IB}(\mathbf{x}) = \sum_{i=1}^N \omega_i \varphi(|\mathbf{x} - \mathbf{x}_i|) + p(\mathbf{x}), \quad (16)$$

where  $\omega_i$  is the weights of the RBF,  $\varphi(|\mathbf{x} - \mathbf{x}_i|)$  is the basis function and the  $r$ th order polyharmonic spline (PHS) functions  $\varphi(r) = r^k \ln(r)$  are used in this work. Applying the orthogonality conditions to close the system, the above can be expressed as a linear system:

$$\begin{bmatrix} M & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \omega \\ \beta \end{bmatrix} = \begin{bmatrix} u \\ 0 \end{bmatrix} \quad (17)$$

where  $[M]_{N \times N} = \varphi(|\mathbf{x}_i - \mathbf{x}_j|)$  and  $P = [1, \mathbf{x}_i^T]$ . In practice, (17) is solved by the external library *LAPACK*. Once the weights are known, a matrix-vector multiplication can be performed for getting the final  $u_{IB}$ . It is also worth noting that the RBFs weights are computed once at the beginning of the simulation as a pre-processing step.

## III. RESULTS AND DISCUSSION

### A. Convergence test for Dirichlet boundary condition

Firstly, the spectral SPH discretization scheme is tested through calculating the gradient operators of two 2D test functions satisfying Dirichlet boundary condition. One is a sinusoidal function  $f(\mathbf{x}) = \sin(2\pi x) \sin(2\pi y)$  and the other is a more general 9th order polynomial  $f(x, y) = 14(x^9 + y^9) - 63(x^8 + y^8) + 140(x^7 + y^7) - 168(x^6 + y^6) + 105(x^5 + y^5) - 35(x^4 + y^4) + 6(x^3 + y^3) - 0.5(x^2 + y^2) + 0.5(x + y)$ . The high order G4 and G6 kernel function is used for the interpolation, and the  $L_2$  norm will be studied to indicate the order of accuracy of the proposed spectral SPH scheme. It can be seen in Fig. 1 that the proposed spectral SPH scheme can achieve the expected order of accuracy (4th and 6th) for Dirichlet boundary condition in the inner fluid region.

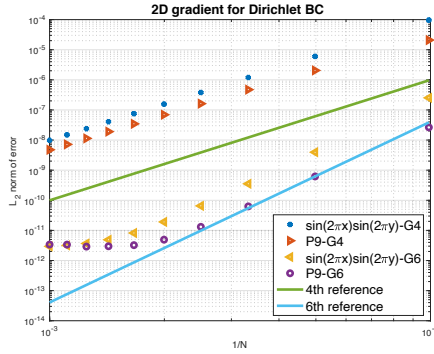


Fig. 1: Convergence result of spectral gradient of 2D test functions satisfying Dirichlet boundary condition.

### B. Numerical test of the 2D SPH solver

In this section, we choose a 2D flow past periodic cylinders problem to demonstrate the oscillation-free characteristic of the scheme. It has been extensively studied as a simplified model of flow through porous media by using combined IBM/spectral method [7]. To solve this problem by spectral SPH, a single cylinder with the radius  $r = 0.02$  m is located in the middle of a square domain of  $L = 0.1$  m as shown in Fig. 2. The flow is initially at rest and driven by a horizontal body force  $F = 1.5 \times 10^{-5}$  m/s<sup>2</sup> until the steady state has been reached. The kinematic viscosity is  $10^{-6}$  m<sup>2</sup>/s which will result in  $Re = 100$ . In order to simulate the indefinite arrays of cylinders, periodic boundary conditions are implemented in both  $x$  and  $y$  direction which also makes the Fourier basis function applicable. We reserve the DTT implementation for future works. All the

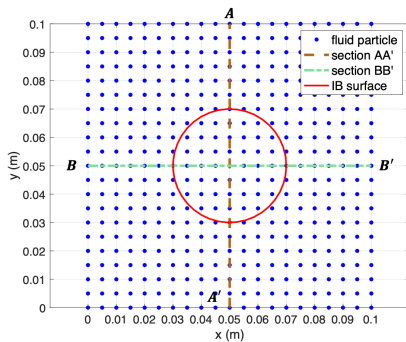


Fig. 2: Geometry of flow past periodic cylinder. (Section  $A - A'$  is the vertical line and section  $B - B'$  is the horizontal line.)

current results are compared with results in [7] at  $t = 200$  s where the steady state has been reached. The pressure profile along section  $B - B'$  can be found in Fig. 3. It can be seen that spectral SPH with RBF extrapolation agrees well with the reference results, providing an oscillation-free pressure profile, while IBM-simple scheme has oscillations in the fluid region.

## IV. CONCLUSION

This paper presents a novel spectral SPH scheme for different boundary conditions. The approach proposed here is based on performing both the spatial differentiation and the solution of the PPE in spectral space. Moreover, an RBF-IBM method is implemented into the scheme to allow an accurate and oscillation-free solution for the simulations with complex solid boundaries. The high order of convergence and the oscillation-free characteristic of the scheme has been validated through CFD benchmark. Future work will be focused on validating wall boundary conditions through the DTT-based Navier-Stokes solver.

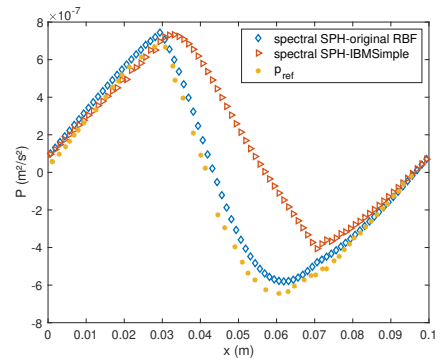


Fig. 3: Pressure profiles through section  $B - B'$  at  $t=200$  s through different spectral SPH-IBM schemes.

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