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Compact moving least squares: An optimization framework for generating high-order compact meshless discretizations

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ABSTRACT

A generalization of the optimization framework typically used in moving least squares is presented that provides high-order approximation while maintaining compact stencils and a consistent treatment of boundaries. The approach, which we refer to as compact moving least squares, resembles the capabilities of compact finite differences but requires no structure in the underlying set of nodes. An efficient collocation scheme is used to demonstrate the capabilities of the method to solve elliptic boundary value problems in strong form stably without the need for an expensive weak form. The flexibility of the approach is demonstrated by using the same framework to both solve a variety of elliptic problems and to generate implicit approximations to derivatives. Finally, an efficient preconditioner is presented for the steady Stokes equations, and the approach's efficiency and high order of accuracy is demonstrated for domains with curvi-linear boundaries.

1. Introduction

Meshless methods have long presented a promising Lagrangian framework for simulating flows with complex moving geometries and moving interfaces, but have failed to gain traction as a high-order method due to a lack of efficient quadrature rules for rational functions, the large support of high-order basis functions, and deficiencies in approximation near boundaries. The current work stems from an attempt to extend the flexibility of low-order meshless approaches to solve Lagrangian hydrodynamics [1] to high order using the moving least squares (MLS) framework [2]. MLS provides a simple and rigorous approach to achieve high-order reconstruction, but the previous list of challenges prevent their stable and efficient application to standard pressure projection schemes. The modified framework that we present here, which we refer to as compact moving least squares (CMLS), remedies these issues while generalizing classical compact finite difference schemes.

Classical compact finite difference methods (CFDM) achieve accuracy competitive with spectral/hp-element methods by exploiting symmetry in the stencil and knowledge of derivatives of the underlying function, obtained either by tailoring the reconstruction to incorporate information from the PDE [3] or by developing implicit formulas for derivatives [4]. We recall fundamental properties of these classes of schemes in Section 2. By exploiting this additional information, high-order polynomial reproduction can be obtained using a small number of neighbors per particle, but these schemes require equispaced neighbors to analytically derive stencils from Taylor series. For a general distribution of nodes, multivariate interpolation of nodal data is in general not possible and moving least squares (MLS) and radial basis functions (RBF) have emerged as the

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two leading methods for robust high-order meshless approximation on general datasets [5]. For lower order approximation, smooth particle hydrodynamics (SPH) has been established as the oldest meshless method for a variety of problems, despite technical challenges regarding numerical instabilities and a lack of even zeroth order consistency in some formulations of the method. By introducing kernel corrections to enforce linear consistency, several approaches achieve second-order convergence, but lose the conservation properties of SPH. These corrections lead to a discretization that in some ways resembles low-order MLS/RBF finite difference methods [1,6].

The current approach will present an optimization framework that introduces a regularization to incorporate Hermite data into the MLS process, generalizing the CFDM method to arbitrary particle distributions. The stencils generated using this approach behave in a manner identical to CFDM: we will demonstrate that, provided a solution to the optimization problem can be stably computed, for problems with smooth solutions the discretization is consistent and convergence is obtained up to the order of polynomial used in the MLS reconstruction and easily preconditioned with standard techniques. In comparison to SPH methods, we demonstrate that for the support typically used to discretize the Laplacian when simulating viscous flow [7], the CMLS method is able to attain a sixth order discretization. This is relevant to a recent trend in which implicit projection methods are used to simulate Lagrangian hydrodynamics in the incompressible SPH (ISPH) methods (see e.g. [8–12]), where our new discretization can be used to achieve substantially higher order convergence while avoiding challenges associated with consistent enforcement of boundary conditions.

In the RBF community, generalizations of the finite difference radial basis function method (RBF-FD) employ a similar strategy using information gleaned from the underlying PDE to achieve compact discretizations (e.g. [13–16]). While our approach is similar in broad strategy, posing the reconstruction as an ℓ_2-optimization allows a flexible framework that can make use of the wealth of information regarding stable solution of least squares problems in the literature [17,18] and a simplified analysis; assuming that for a given particle distribution a local polynomial reconstruction exists, the existence of an MLS reconstruction follows from standard convex optimization arguments [5,19]. We will show that an optimization framework allows boundary conditions to be enforced locally via equality constraints without introducing global penalty parameters. While for simplicity in this work we present a polynomial reconstruction, in principle the reconstruction space can be enriched with any test functions (possibly singular). Additionally, although RBF-type approaches have successfully generalized CFDM schemes resembling [3], to our knowledge the current approach marks the first method that allows implicit formulas for differential operators generalizing Lele-type schemes [4]. To this end, we claim that this approach is therefore more flexible, and we provide evidence that we are able to obtain $O(N)$ results for both implicit approximation of derivatives and for the monolithic solution of the steady Stokes equations.

We begin by providing a brief review of compact finite difference methods in Section 2 and of classical moving least squares in Section 3 before introducing the CMLS method in Section 4. We demonstrate recovery of original Lele-type implicit derivatives in Section 5 and proceed in Section 6 by presenting simple examples to demonstrate how the method can be used to solve Poisson and Helmholtz problems in 1D and 2D. We then demonstrate the necessity of our novel boundary condition approach in performing Helmholtz decompositions as would be used in a projection method for solving fluid mechanics problems. We finally use the framework to solve the monolithic Stokes equations in Section 7 and present a block preconditioner that is able to solve the resulting system with $O(N)$ complexity while recovering optimal convergence.

2. Compact finite differences

In compact finite differences, there are two broad strategies which we will refer to as Weinan-type schemes [3] and Lele-type schemes [4]. We will later show that the CMLS schemes generalize both of these approaches for unstructured stencils and arbitrary order.

In the Weinan-type schemes, the PDE is used together with exact expressions for truncation error to achieve fourth-order compact stencils. Consider the solution of the Poisson problem $u'' = f$ on a periodic domain in 1D. To discretize the second derivative a standard centered difference is used

$$u_i'' \approx D_{xx}u = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u_i'' + Ch^2 u_i'''' + O(h^4) \tag{1}$$

where C is a constant that can be calculated exactly using Taylor series. The PDE can be used to eliminate the second order term in the truncation error

$$Ch^2 u_i'''' = Ch^2 f_i'' \approx Ch^2 D_{xx} f + O(h^4) \tag{2}$$

and after reorganizing, a fourth order expression for the second derivative is obtained with the same bandwidth as the centered difference.

$$D_{xx}^{compact} u_i = D_{xx}u_i - Ch^2 D_{xx} f_i = u_i'' + O(h^4) \tag{3}$$

This approach requires that C be calculable, which is trivial for uniform grids. In Lele-type schemes, implicit expressions for derivatives are sought of the form

$$\sum_{j=-N}^{N} \alpha_j u'_{i+j} = \frac{\sum_{j=1}^{M} a_j \left(u_{i+j} - u_{i-j}\right)}{h} + O(h^{Q+1}) \tag{4}$$