Multiscale Flow Simulation by Adaptive Finite Volume Particle Methods

Armin Iske[*1]

[1] Department of Mathematics, University of Leicester, Leicester LE1 7RH, UK

We report on recent developments concerning adaptive finite particle methods, which are used for the numerical simulation of multiscale phenomena in time-dependent evolution processes. The proposed concept relies on a finite volume approach, which we combine with WENO reconstruction from particle average values. In this method, polyharmonic splines are key tools for both the optimal recovery from scattered particle averages and the construction of customized adaption rules.

1 Introduction

Many physical phenomena in fluid dynamics are modelled by time-dependent scalar hyperbolic conservation laws of the form

$$\frac{\partial u}{\partial t} + \nabla f(u) = 0, \tag{1}$$

where for some domain $\Omega \subset \mathbb{R}^d$, $d \geq 1$, and a time interval $I = [0, T]$, $T > 0$, the unknown function $u : I \times \Omega \to \mathbb{R}$ measures the density of some conserved quantity, such as mass, momentum, or energy. In nonlinear conservation laws, i.e., for nonlinear flux function $f(u) = (f_1(u), \ldots, f_d(u))$, the solution u of (1) can easily develop discontinuities (shocks) spontaneously, even from smooth initial data

$$u(0, x) = u_0(x), \qquad \text{for } x \in \Omega. \tag{2}$$

This typical behaviour reflects problem-inherent *multiscale phenomenona*, which must be dealt with mathematically and computationally, where *adaptive* simulation methods are essentially needed for solving the Cauchy problem (1),(2).

Moreover, due to irrevocable laws of physics, a numerical method for the solution of (1) is required to be conservative. Finite volume (FV) discretizations are classical conservative methods for hyperbolic problems [9]. In the general formulation of FV, the computational domain Ω is partitioned into disjoint grid cells, control volumes. However, as shown by Junk in [7], FV methods can also be formulated without using a grid. In fact, a very flexible and robust *finite volume particle method* (FVPM) is developed in [3] by Hietel, Steiner and Struckmeier, where the control volumes in the FV method are replaced by *influence areas* of moving particles. To this end, a partition of unity is used, which also allows overlapping influence areas.

In this short contribution, we adopt only some of the basic ideas of FVPM (see Section 2), which we combine with both *weighted essentially non-oscillatory* (WENO) reconstruction (Section 4) and a customized adaption strategy for the particles' local refinement and coarsening (Section 5). This altogether yields a novel concept for multiscale flow simulation by adaptive particle methods, which relies on scattered data reconstruction by using polyharmonic splines (Section 3).

We remark that the good performance of related multiscale particle simulation methods is already demonstrated in our previous work concerning two-phase flow in porous media. Therefore, for the (required) sake of brevity, we refrain from including numerical examples, but refer to the numerical results and comparisons in our previous work [5] and [6, Chapter 11].

2 Finite Volume Particle Method

In order to briefly explain the main ingredients of the utilized finite volume particle method (FVPM), let $\Xi = \{\xi\}_{\xi \in \Xi} \subset \Omega$ denote a finite set of nodes, each of which corresponding, at a time $t \in I$, to one flow particle. Moreover, we denote for any $\xi \in \Xi$ by $V_\xi \subset \Omega$ the *influence area* of particle ξ, with *particle average*

$$\bar{u}_\xi(t) = \frac{1}{|V_\xi|} \int_{V_\xi} u(t, x)\, dx, \qquad \text{for } \xi \in \Xi \text{ and } t \in I.$$

According to the classical concept of FV [9], for each $\xi \in \Xi$ its particle average $\bar{u}_\xi(t)$ is at time step $t \to t + \tau$ updated by an explicit numerical method of the form

$$\bar{u}_\xi(t + \tau) = \bar{u}_\xi(t) - \frac{\tau}{|V_\xi|} \sum_\nu F_{\xi,\nu},$$

where $F_{\xi,\nu}$ denotes the *numerical flux* between particle ξ and a neighbouring particle $\nu \in \Xi \setminus \xi$. The required exchange of information between neighbouring particles is modelled via a generic numerical flux function, which may be implemented by using any suitable FV flux evaluation scheme, such as ADER in [8]. For details on further features of FVPM, see [3, 7].

* Corresponding author: e-mail: iske@mcs.le.ac.uk, Phone: +44(0)116 252 3899, Fax: +44(0)116 252 3915

3 Optimal Recovery from Particle Averages by Polyharmonic Splines

On given particle averages $\bar{u}\big|_{\Xi} = \{\bar{u}_\xi\}_{\xi\in\Xi}$, and for specific *stencils* (see Section 4), WENO reconstruction requires computing for each stencil $\mathcal{S} \subset \Xi$ a recovery function $s : \mathbb{R}^d \to \mathbb{R}$ satisfying $\bar{u}_\xi = \bar{s}_\xi$ for all $\xi \in \mathcal{S}$. Commonly used WENO schemes work with polynomial reconstruction, which, however, may lead to severe numerical instabilities, especially when the particles are heterogeneously distributed, see [1]. Our recommendation is to rather work with polyharmonic splines, in which case

$$s(x) = \sum_{\xi\in\Xi} c_\xi \bar{\phi}^{m,d}_\xi(\|x - \cdot\|) + p(x), \qquad p \in \mathcal{P}^d_m, \tag{3}$$

where $\mathcal{P}^d_m$ are the d-variate polynomials of order at most m, and where, for $2m > d$, the *polyharmonic spline* $\phi^{m,d}$ is given by $\phi^{m,d}(r) = r^{2m-d}\log(r)$ for even dimension d, and by $\phi^{m,d}(r) = r^{2m-d}$ for odd dimension d.

We remark that polyharmonic splines, discovered by Duchon [2], are powerful tools for multivariate interpolation from scattered Lagrange data. As shown in [4], polyharmonic spline interpolation can be generalized to reconstruction from scattered Hermite-Birkhoff data, which includes reconstruction from particle averages. Moreover, polyharmonic spline reconstruction is *optimal* in the *Beppo Levi space* $\mathrm{BL}^m(\mathbb{R}^d) = \left\{u : D^\alpha u \in L^2(\mathbb{R}^d) \text{ for all } |\alpha| = m\right\}$, being equipped with the semi-norm

$$|u|^2_{\mathrm{BL}^m} = \sum_{|\alpha|=m} \binom{m}{\alpha} \|D^\alpha u\|^2_{L^2(\mathbb{R}^d)},$$

so that s in (3) minimizes the Beppo Levi energy $|\cdot|_{\mathrm{BL}^m}$ among all recovery functions u in $\mathrm{BL}^m(\mathbb{R}^d)$, i.e., $|s|_{\mathrm{BL}^m} \le |u|_{\mathrm{BL}^m}$.

4 WENO Reconstruction

WENO reconstruction requires first selecting, for any particle $\xi \in \Xi$, a small number of stencils $\mathcal{S}_i \subset \Xi$, $1 \le i \le k$, each given by a small set of particles in the neighbourhood of ξ. For each stencil $\mathcal{S}_i$, we compute a polyharmonic spline reconstruction s_i satisfying $\bar{u}\big|_{\mathcal{S}_i} = \bar{s_i}\big|_{\mathcal{S}_i}$, so that the approximation s to u in the influence area V_ξ of particle ξ is given by a weighted sum of the form

$$s(x) = \sum_{i=1}^k \omega_i s_i(x), \qquad \text{with } \sum_{i=1}^k \omega_i = 1,$$

where the weights $\omega_i = \tilde{\omega}_i \big/ \sum_{j=1}^k \tilde{\omega}_j$, with $\tilde{\omega}_i = (\epsilon + \mathcal{I}(s_i))^{-\rho}$ for $\epsilon, \rho > 0$, are determined by using the *oscillation indicator*

$$\mathcal{I}(u) = |u|^2_{\mathrm{BL}^m} = \sum_{|\alpha|=m} \binom{m}{\alpha} \|D^\alpha u\|^2_{L^2}, \qquad \text{for } u \in \mathrm{BL}^m(\mathbb{R}^d).$$

5 Adaption Rules

In order to construct customized adaption rules, we employ an *error indicator* $\eta : \Xi \to [0, \infty)$ of the form

$$\eta(\xi) = |\bar{u}_\xi - \bar{s}_\xi|, \qquad \text{for } \xi \in \Xi,$$

where s denotes the polyharmonic spline reconstruction satisfying $\bar{u}\big|_{\mathcal{S}} = \bar{s}\big|_{\mathcal{S}}$, for a stencil $\mathcal{S} \subset \Xi\backslash\xi$ of particles surrounding ξ. We let $\eta^* = \max_{\xi\in\Xi} \eta(\xi)$, and we determine relative threshold values $\theta_{\mathrm{crs}}, \theta_{\mathrm{ref}}$, $0 < \theta_{\mathrm{crs}} < \theta_{\mathrm{ref}} < 1$, so that a particle $\xi \in \Xi$ is *to be refined*, iff $\eta(\xi) > \theta_{\mathrm{ref}} \times \eta^*$, wheras ξ is *to be coarsened*, iff $\eta(\xi) < \theta_{\mathrm{crs}} \times \eta^*$. It is sufficient for the purpose of this short contribution to say that a particle $\xi \in \Xi$ is coarsened by its removal from Ξ, whereas ξ is refined by the insertion of further particles in its neighbourhood. For further details concerning computational aspects of the utilized adaption rules and their construction, we refer to our previous papers [5, 8].

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