Anisotropic kernels for self-organizing Lagrangian particles

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ABSTRACT

Lagrangian particle methods are powerful numerical tools for simulating convection-dominated problems and problems in complex geometries. The method is adaptive, since particles naturally follow the flow map, and the resolution can be locally adapted by changing the core sizes (smoothing lengths) of the particles [2]. Determining the total number of particles required to reach a certain error level, as well as a good placement of the particles in the computational domain, however, is not trivial. Principles from particle self-organization (inverse statistical mechanics) allow automatically finding near-optimal distributions of particles at runtime [4]. Additionally, particles are inserted in under-resolved regions and removed from over-resolved regions in order to ensure consistent function approximation everywhere and to dynamically adapt the total number of particles in the simulation [4].

We approximate derivatives using DC-PSE operators, which have been shown to be consistent on arbitrary particle distributions, as well as near boundaries [6]. Particle sizes and cutoff radii are locally adapted as governed by a resolution monitor function [4]. The approximation error of adaptive-resolution DC-PSE operators is bounded by $|u(x) - u_h^\epsilon(x)| \leq C h_x^m ||u(x)||_{W^m_\infty(B)}$, where $h_x$ is the local inter-particle distance and $||u(x)||_{W^m_\infty(\Omega)} = \max_{|\alpha| \leq m} ||\partial^\alpha u||_{L_\infty(\Omega)}$ is a measure for the magnitude of the derivatives of the function $u$. $B$ is the ball with radius $r_{c,p}$, the local cutoff radius around particle $p$. The integer $m$ is the approximation order. The magnitude of the largest partial derivative in any direction hence determines the maximum error. If the directional derivatives of the function are anisotropic, this motivates the use of anisotropic (“elliptical”) kernels to further reduce the total number of particles required to represent the function, as illustrated in Fig. 1. This is analogous to ideas used in anisotropic-smoothing SPH [3].

Here we present a self-organizing Lagrangian particle method with anisotropic DC-PSE kernels where the scalar kernel width (smoothing length) $\epsilon_p$ of particle $p$ is replaced by a tensor $G_p$ defining the size, anisotropy, and orientation of the kernel at particle $p$. Figure 2 visualizes results from the 2D Burgers equation $\partial_t f + \text{Re} [f, f] \cdot \nabla f = \Delta f$ with initial condition $u(x, y, t = 0) = \cos(2\pi x) \cos(2\pi y)$ and doubly periodic boundary conditions in the computational domain $[0, 1]^2$.

We further describe solutions to technical problems associated with the efficient parallel implementation of self-organizing anisotropic particle methods. This includes adaptive domain decompositions over anisotropic particles, anisotropic halo (ghost) layers, data structures for efficiently finding the interaction partners of anisotropic particles with locally adapted resolution [1], and a potential-minimization algorithm for the self-organization of elliptical particles. The method has been implemented both in 2D and 3D as a client for the distributed-memory parallel computing middleware PPM [5].
Figure 1: Comparison of the particle distributions resulting from self-organization to the gradient of the function $\exp(-50((x-0.5)^2 + (y-0.5)^2))$ in 3D. Color codes the $x$ coordinate for visualization.

Figure 2: Particle distribution (a) and kernel orientation and anisotropy (b) for 1000 self-organizing particles adapting to the solution of the 2D Burgers equation at time $T = 0.126/\text{Re}$ with $\text{Re} = 100$. Color codes the function value $u$.

References


