## Particle Motion and Adaptivity for Meshfree Methods Using an Error Potential Function

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## ABSTRACT

Meshfree methods use particles to serve as nodes and/or quadrature points in a numerical scheme. In many cases, the arrangement is either static or follows the local velocity vector for convective problems. We present an alternative approach in which particles move in response to the numerical aspects of solution rather than the physical aspects of the solution. While motion in particle methods has its origin in avoiding unstable or inaccurate numerical methods to handle convection operators, quantified accuracy is important in many applications when rigorous solution verification is required. While structured arrangements of particles often enable analytical error estimation, this is not the case for unstructured sets of particles. In addition, unstructured arrangements have been empirically observed to have much greater errors.

This work builds upon adaptivity in mesh-based methods (Loseille \& Alauzet 2009, Yano \& Darmofal 2012) to approximate global error functions using local error functions, which are then minimized. To perform the minimization in this context, inspired by molecular dynamics, we approximate the error function using local error terms based on potentials. In this manner, higher error regions are identified when gradients are high and particle densities are low. Regions of high gradients and poor resolution then attract particles. Importantly, the error potentials are anisotropic based on the local principle axes of solution data, e.g. stress tensors. Solutions are obtained by iterating between the discrete PDE and minimization of the error potential. We demonstrate the approach on elliptic and parabolic equations.

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## REFERENCES

- [1] Y. Bourgault, M. Picasso, F. Alauzet, and A. Loseille, "On the use of anisotropic *a posteriori* error estimators for the adaptive solution of 3D inviscid compressible flows", *Int. J. Num. Metho. Engng*, **59**, 47-74 (2009).
- [2] M. Yano and D. Darmofal, "An optimization-based framework for anisotropic simplex mesh adaptation", J. Comp. Phys., 231, 7626-7649 (2012).