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Symmetric quadrature rules for simplexes based on sphere close packed lattice arrangements

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HIGHLIGHTS

- A general approach for computing optimal symmetric quadrature rules on simplexes is identified.
- A new family of optimal symmetric quadrature rules on the 2-simplex (triangle) is identified.
- A new optimal symmetric quadrature rule on the 3-simplex (tetrahedron) is identified.

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ABSTRACT

Sphere close packed (SCP) lattice arrangements of points are well-suited for formulating symmetric quadrature rules on simplexes, as they are symmetric under affine transformations of the simplex unto itself in 2D and 3D. As a result, SCP lattice arrangements have been utilized to formulate symmetric quadrature rules with $N_p = 1, 4, 10, 20, 35$, and 56 points on the 3-simplex (Shunn and Ham, 2012). In what follows, the work on the 3-simplex is extended, and SCP lattices are employed to identify symmetric quadrature rules with $N_p = 1$, 3, 6, 10, 15, 21, 28, 36, 45, 55, and 66 points on the 2-simplex and $N_p = 84$ points on the 3-simplex. These rules are found to be capable of exactly integrating polynomials of up to degree 17 in 2D and up to degree 9 in 3D.

1. Introduction

There have been significant efforts to identify high-order quadrature rules on d-simplex and d-hypercube geometries as evidenced by the surveys in [1–5]. On the d-hypercube, it is well-known that optimal (or near optimal) quadrature rules with $N_p = n^d$ points can be constructed from tensor products of 1D Gauss–Legendre quadrature rules with n points [6]. These quadrature rules are widely used because, in addition to their optimality (or near optimality), they are symmetric (as they are invariant under reflections and rotations that map the d-hypercube unto itself), possess positive weights, and have points located within the interior of the d-hypercube. Due to these desirable properties, there have been attempts to extend the Gauss–Legendre rules to d-simplexes (cf. [6,7]). The simplest of such approaches has involved constructing Gauss–Legendre rules on the d-hypercube and then degenerating vertices until the d-simplex is obtained. However, in general the resulting rules are no longer symmetric on the d-simplex, as they contain anisotropic clusters of points near the degenerate vertices. In addition, the optimality of these rules has yet to be shown analytically. In fact, to the authors' knowledge, no one has identified a family of symmetric quadrature rules on the d-simplex for which optimality can be rigorously proven. For this reason, the formulation of quadrature rules on the d-simplex remains an open area of research, as demonstrated by the recent work presented in [8–17].

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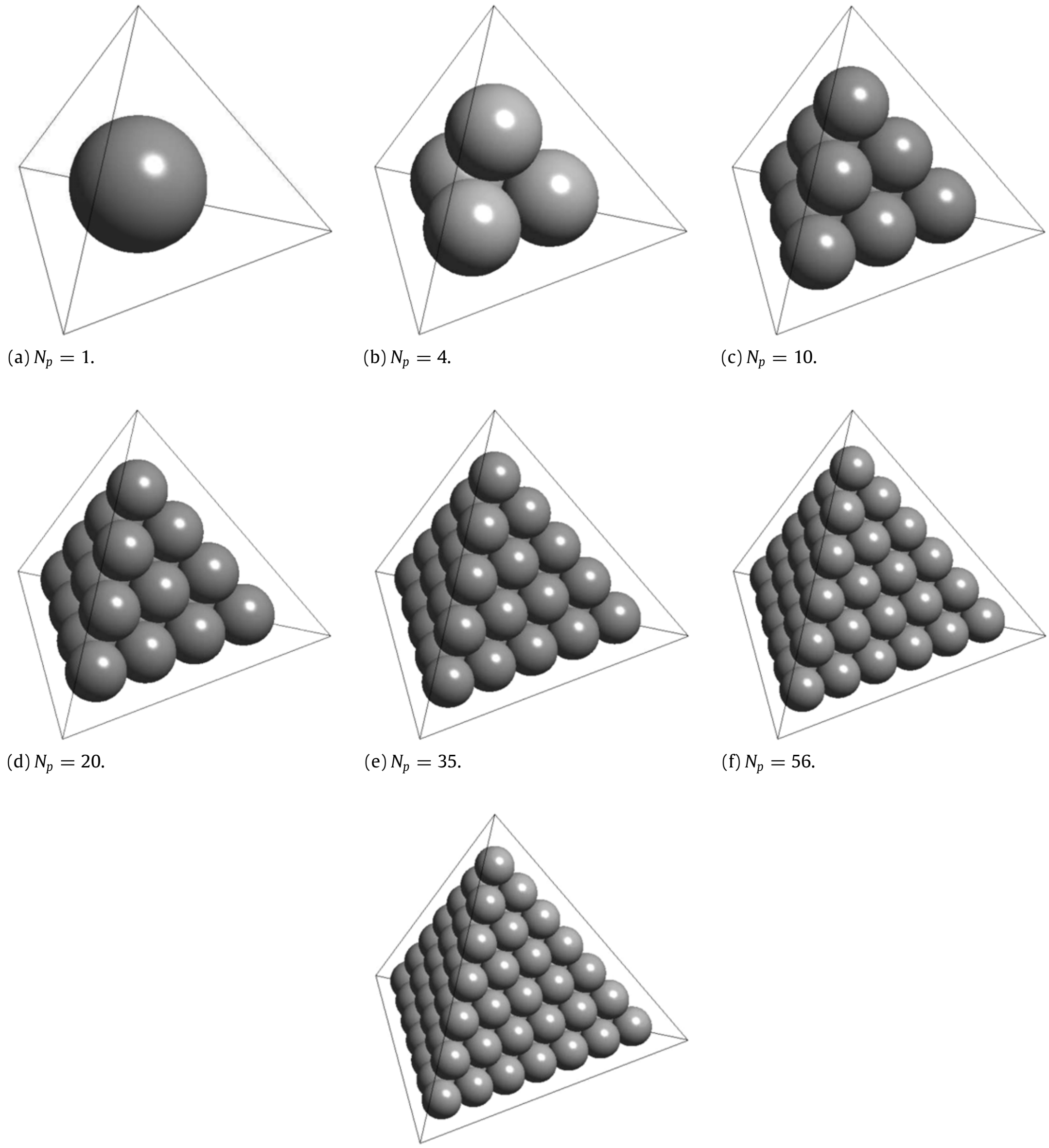

(a) $N_p = 1$.
(b) $N_p = 4$.
(c) $N_p = 10$.
(d) $N_p = 20$.
(e) $N_p = 35$.
(f) $N_p = 56$.
(g) $N_p = 84$.

Fig. 1. Cubic close packed (CCP) configurations on tetrahedra with $N_p = 1, 4, 10, 20, 35, 56$, and 84 points.

Of particular interest, is the effort by Shunn and Ham in [17] to construct quadrature rules on the 3-simplex based on cubic close packing (CCP) arrangements of points. In their work, the CCP arrangements of points (i.e., the CCP lattices) are defined by the centers of spheres in the CCP configuration, as shown in Fig. 1 for the cases of $N_p = 1, 4, 10, 20, 35, 56$, and 84.

The CCP lattices are viewed as the 3-simplex analog to the uniform cartesian lattices on which the Gauss–Legendre rules on the 3-hypercube are based, in the sense that they possess the same properties of symmetry on the 3-simplex as uniform cartesian lattices possess on the 3-hypercube. Based on this fact, it was supposed that an optimal family of symmetric quadrature rules on the 3-simplex could be obtained by employing the CCP lattices as initial conditions to optimization procedures for identifying the rules. Following this approach, a family of symmetric, locally optimal quadrature rules on the 3-simplex with $N_p = 1, 4, 10, 20, 35$, and 56 points was obtained [17].

This work attempts to extend the approach in [17] to identify new quadrature rules on the d-simplex for the cases of $d = 2$ and $d = 3$. This extension requires the construction of CCP lattices in 2-space (sometimes referred to as 'hexagonal packing lattices'), which are shown in Fig. 2 for the cases of $N_p = 1, 3, 6, 10, 15, 21, 28, 36, 45, 55$, and 66.

For convenience, the analogs of the CCP lattices in d-space will henceforth be referred to as d-sphere close packed lattices (d-SCP lattices). It is useful to note that, in general, the number of points in the d-SCP lattices (the values of N_p for the lattices)