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Molecular dynamics-based unstructured grid generation method for aerodynamic applications

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HIGHLIGHTS

- Triangular mesh generation based on the molecular dynamics method is developed.
- Mesh adaptation technology for molecular dynamics simulation is suggested.
- Suggested algorithm works identically for 1D, 2D and 3D problems.
- Computational grids have been tested for hypersonic flow past unmanned airplane X-43.

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ABSTRACT

A new approach to triangular mesh generation based on the molecular dynamics method is proposed. Mesh nodes are considered as interacting particles. After the node placement by molecular dynamics simulation, well-shaped triangles or tetrahedra can be created after connecting the nodes by Delaunay triangulation or tetrahedrization. Some examples are considered in order to illustrate the method's ability to generate a mesh for an aircraft with a complicated boundary. Mesh adaptation technology for molecular dynamics simulation is presented.

1. Introduction

The concept of a mesh as a discretization of space has been associated with computational methods since the first attempts to obtain numerical solutions of partial differential equations. Establishing a suitable mesh is a rather tedious exercise and a minor part of the computational effort involved in solving partial differential equations by either a finite difference or finite element method.

Although a mesh is a prerequisite for numerical computation in many areas of science and engineering, it was computational fluid dynamics, and computational aerodynamics in particular, that were the key drivers in stimulating the development of reliable and efficient mesh generators.

The accuracy of the flow simulations based on the Reynolds averaged Navier Stokes (RANS) equations over the complete aircraft is influenced by many factors: discretization formulas for the flow equations which introduce only minimal amounts of artificial dissipation, a turbulence model that captures the boundary layer behavior, a flow solver that will achieve a high degree of convergence, and, finally, a mesh that has good quality and is sufficiently fine to permit a good approximation of the flow solution throughout the region of interest.

Unstructured grids are widely used in computational aerodynamics in spite of the fact that predictions based on the RANS equations using a structured (i.e. hexahedral) mesh are generally higher, and closer to the experimental values, than comparable predictions on an unstructured mesh of tetrahedra.

Unstructured grids have significant advantages:

- The advantage of unstructured grid methods is that they have the ability to be automated to a large degree and, therefore, require little user time or effort. The user need not worry about laying out block structure or connections. Additionally, unstructured grid methods are well suited to inexperienced users because they require little user input and will generate a valid mesh under most circumstances. Unstructured methods also enable the solution of very large and detailed problems in a relatively short period of time. Grid generation times are usually measured in minutes or hours.

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- Unstructured grids have the advantage of generality in that they can be made to conform to nearly any desired geometry. Grid has a great flexibility in handling complex geometries.
- These grids tend to be easier to generate than structured or composite multiblock grids.
- The multiblock structured mesh generation technique requires definition and discretization of the block interfaces. A good graphics user interface (GUI) can ease the burden of creating the block structure, but it can still be a largely manual task and time consuming process. Therefore multiblock grid generation times are usually measured in days if not weeks. More significantly, the difficulty of automating this process inhibits the use of composite block methods for solving time evolving problems, or other situations such as automatic design, where the boundary shape is changing.

This generality, however, comes with a price:

- The major drawback of unstructured grids is the lack of user control when laying out the mesh. Typically any user involvement is limited to the boundaries of the mesh with the mesher automatically filling the interior.
- Triangle and tetrahedral elements have the problem that they do not stretch or twist well; therefore, the grid is limited to being largely isotropic, i.e. all the elements have roughly the same size and shape (great difference in neighboring element sizes can increase numerical approximation errors). This is a major problem: when trying to refine the grid in a local area, often the entire grid must be made much finer in order to get the point densities required locally.
- Another drawback of the methods is their reliance on good CAD data. Most meshing failures are due to some (possibly minuscule) error in the CAD model.
- Unstructured grids require more information to be stored and recovered than structured grids (e.g., the neighbor connectivity list). Unstructured flow solvers typically require more memory and have longer execution times than structured grid solvers on a similar mesh.
- Post-processing the solution on an unstructured mesh requires powerful tools for interpolating the results onto planes and surfaces of rotation for easier viewing.
- Unstructured grid methods generally have poorer numerical accuracy. For example, it is difficult to construct approximations that maintain an accurate propagation of one-dimensional flow disturbances because tetrahedral grid elements have no parallel faces.

There are several essentially different approaches to generating triangular or tetrahedral meshes. The most common of these are the moving front technique [1,2] and Delaunay based methods [3–12].

The moving front technique starts from a prescribed boundary definition (set of edges in 2D, set of triangular faces in 3D) which remains intact throughout the mesh generation process. The boundary triangulation is regarded as a front on which a new layer of elements is built. The original front triangles become interior faces of the mesh and a new set of front faces is created, a process that continues until the entire domain has been filled.

The majority of Delaunay based methods exploit an incremental algorithm that starts with an initial triangulation of just a few points [7,8]. The complete triangulation is generated by introducing points and locally reconstructing the triangulation after each point insertion.

In contrast to the approach of incrementally inserting nodes one by one into an existing mesh, some mesh generation methods place all the nodes first before connecting them into a mesh. Nodes are first distributed into optimal locations to cover the whole domain, and then connected into mesh. In the bubble meshing method [13], Shimada and Gossard place nodes at centers of a set of packed spheres or bubbles. An inter-bubble force function is defined between adjacent bubbles, a force balancing configuration of the nodes is found by performing dynamic simulation. After node placement, the method connects the nodes into well-shaped mesh elements by constrained Delaunay triangulation or tetrahedrization. In [14] Persson and Strang treat a simplex mesh as a truss structure and mesh points as nodes of the truss. A linear force–displacement function is defined for each pair of nodes connected by a bar (or edge). Nodes are gradually moved to optimal locations by iteratively solving for force equilibrium. At each iteration, the node set is re-triangulated using the Delaunay triangulation algorithm in order to decide the edges. In the end, a high quality triangular mesh is obtained.

In study [15] surface or volume geometries to be meshed are treated as atomic systems, and mesh nodes are considered as interacting particles. By minimizing system potential energy with Monte Carlo simulation, particles are placed into a near optimal configuration. Well-shaped triangles or tetrahedra can then be created after connecting the nodes by constrained Delaunay triangulation or tetrahedrization.

The isosurface stuffing algorithm is presented in [16] that fills an iso-surface with a uniformly sized tetrahedral mesh whose dihedral angles are bounded between 10.7° and 164.8°. The algorithm is fast, numerically robust, and easy to implement because it generates tetrahedra from a small set of pre-computed stencils. A variant of the algorithm creates a mesh with internal grading: on the boundary, where high resolution is generally desired, the elements are fine and uniformly sized, but in the interior they may be coarser and vary in size. The isosurface stuffing method is a powerful tool for dynamic fluid simulation, large-deformation mechanics, and applications that require interactive remeshing or use objects defined by smooth implicit surfaces. The algorithm is perfect for robust remeshing in physically-based animation at interactive rates.

In paper [17] Nochetto and Walker presented a hybrid variational front tracking-level set method for generating 2D unstructured triangular meshes that undergo large deformations and topological changes in an automatic way. The method is based on the idea of combining the level set and front-tracking methods. The level set method advects a scalar field function whose zero level set represents the interface and has the advantage of being completely Eulerian and can automatically handle topological changes. The front-tracking method uses an explicit representation of the interface, such as an interface mesh or marker particles to "track" the interface. This hybrid approach combines the accuracy of the explicit mesh methods with the ease of topological transformation to generate meshes of arbitrary domains. In addition, authors introduce a shape optimization approach for ensuring mesh conformity. The method is advantageous for Arbitrary Lagrangian–Eulerian (ALE) type methods and directly allows for using a variational formulation of the physics being modeled and simulated, including the ability to account for important geometric information in the model (such as for surface tension driven flow). The meshing procedure is not required at every time-step and the level set update is only needed during a topological change. Hence, the method does not significantly affect the computational cost.

Our method is not so fast due to the fact that molecular dynamics simulations are inherently time-consuming and computationally expensive and is not applicable for problems requiring interactive remeshing. The molecular dynamics method was developed for mesh generation mainly for aerodynamic problems which do not need frequent remeshing. However, our method is very convenient for relatively rapid local remeshing which is used to solve aerodynamic shape optimization problems. Moreover, in