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Design of adaptive unstructured grids using differential methods

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Adaptive generation of computational grids can improve the efficiency of mathematical modeling by increasing the accuracy of numerical approximations. The paper describes a method for constructing unstructured grids with adaptation based on differential methods. The application of these methods ensures a smooth distribution of the geometric characteristics of the grid, i.e. the appearance of adjacent cells that differ greatly in size and shape becomes unlikely. To achieve proper adaptation in unstructured grids we use the novel approach based on methodology of adaptive structured grid construction. This approach uses the method of grid construction based on solving inverted Beltrami equation to create mapping of some sample grid domain to the physical area. This mapping is used to construct point set on which the unstructured grid is constructed using Delaunay triangulation method. Thus, the result is unstructured grid with proper adaptation. Adding fault and fractures or other structure elements may be supported by implementing constrained Delaunay triangulation.
Key words: computational grid construction algorithm, unstructured mesh, adaptive mesh, differential elliptic equations, reversed Beltrami equation

Дифференциалды әдістерді қолданып бейімделген құрылымдық емес торларды құру

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Есептеуіш бейімделген торларды жасау сандық аппроксимация дәлдігін арттыру арқылы математикалық модельдеудің тиімділігін арттырады. Мақалада дифференциалды әдістерге негізделген бейімделген құрылымдық емес торларды құру әдісі сипатталған. Осы әдістерді қолдану тор ұяшықтарының геометриялық сипаттамаларының тегістелуін қамтамасыз етеді, яғни бұл жағдайда көрші ұяшықтардың көлемдері мен пішіндері тым ұқсамау мүмкіндігі өте төмен.Құрылым сақтамайтын торларда дұрыс бейімделуді қамтамасыз ету үшін адаптивті құрылымдық торларды құру әдістемесіне негізделген жаңа тәсіл қолданылады. Бұл тәсілде керіленген Белтрами теңдеуін шешуге негізделген торларды құру әдісі белгілі бір анықтамалық аймақты физикалық түрде картаға бейнелеуді табу үшін пайдаланылады. Осы салыстыруды пайдалана отырып, Делоне триангуляция әдісін пайдаланып құрылым сақтамайтын тор құру үшін пайдаланылатын нүктелер жиынтығы жасалады. Осылайша, нәтиже дұрыс бейімделуі бар құрылым сақтамайтын тор болып табылады. Жарықтар және сынықтар немесе басқа да құрылымдық элементтерді қосу шектеулері бар Делоне триангуляциясының көмегімен жүзеге асырылады.
Түйін сөздер: Есептеу торын құру алгоритмі, құрылымдық емес тор, бейімделген тор, дифференциалдық эллиптикалық теңдеулер, керіленген Белтрами теңдеуі.

Разработка адаптивных неструктурированных сеток с помощью дифференциальных методов

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Генерация вычислительных адаптивных сеток может повысить эффективность моделирования за счет повышения точности численной аппроксимации. В статье описывается метод построения неструктурированных сеток с адаптацией на основе дифференциальных методов. Применение этих методов обеспечивает плавное распределение геометрических характеристик ячеек сетки, то есть возможность появления соседних ячеек, которые сильно отличаются по размеру и форме, является крайне низкой. Для обеспечения надлежащей адаптации в неструктурированных сетках используется новый подход, основанный на методологии построения адаптивных структурированных сеток. В этом подходе используется метод построения сеток на основе решения обращенного уравнения Бельтрами для создания отображения некоторой эталонной области в физическую. С помощью этого отображения строится набор точек, который будет использован для построения неструктурированной сетки методом триангуляции Делоне. Таким образом, результатом является неструктурированная сетка с хорошей адаптацией. Добавление разломов и трещин или других структурных ограничивающих элементов поддерживается путем реализации триангуляции Делоне с ограничениями.
Ключевые слова: алгоритм построения расчетных сеток, неструктурированная сетка, адаптивная сетка, дифференциальные эллиптические уравнения, обращенное уравнение Бельтрами.

1 Introduction

Adaptation methods for computational grid generation improve the efficiency of physical simulations. They increase accuracy of numerical approximations, because most industrial computational processes have big changes of physical values in some parts of domain. It leads to high gradients and values of solution in those locations which, in turn, leads to lack of accuracy.

Generally grids constructed to numerical solving of partial differential equations are grouped into two essential groups: structured and unstructured grids [1]. Each of those groups has its own construction methodology and fields of use which is almost does not intersect. However, some theoretical principles that may be implemented to overall numerical grids let us consider comparing and combining those methods. One of those is adaptation of the grids.

Adaptive grids allow researchers to avoid creating fine grids for the whole domain. Such grids critically increase computational run time. In many cases locations with smooth solution does not need such surplus accuracy, since it does not take effect considering bad accuracy of places with high gradients of solution.

Computational grids can be constructed in such a way that the places of such big solution values and gradients are covered with small cells. It reduces the error of numerical solution generated in the locations of steep gradients and high values. The grid on the smooth solution locations is coarsened to optimize the computation time. Computational grids are grouped into fundamentally different types of grids called structured and unstructured grids. Both of them have own grid construction methodology.

Unstructured grids are widely used in finite element and finite volume methods. They are necessary in certain situations and have a several benefits comparing to structured grids in case of complicated shapes of domain. Mostly such grids are constructed by geometric and graph methods. The adaptation in those methods are done by adding additional points in the certain locations of the grid.

Common structured grids usually used in finite difference methods are constructed using simple algebraic methods. But the construction gets complicated in situations of adaptation to physical area boundaries and control functions. In such case the structured grid represents curvilinear coordinate system and found by solving non-linear differential equations.

The paper describes grid construction method that has positive characteristics of both approaches by combining them in one method. Combination implemented by constructing unstructured grid based on set of points uniformly scattered over the curvilinear structured grid. In such method the result grid is unstructured grid and, therefore, have all its positive sides. It also keeps the smooth adaptation based on differential methods.

2 Literature review

Most of unstructured grid generation algorithms [2] have 3 groups separated by general approach to construction. First group is advancing front algorithms [3, 4]. In such algorithms they grid is constructed by attaching new cells to the existing grid starting from boundaries of the domain. Next approach is iterative construction of Delaunay triangulation by adding new points to the existing triangulation [5, 6]. After adding the new point whole triangulation is to be reconstructed to satisfy principle of Delaunay. Algorithms based on tree containers such as quadtree algorithms [7, 8]. In such algorithms the forms of the result grid cells may be far from perfect. However this approach allows very convenient adaptation of grid in terms of cell fining.

These approaches may be improved to support constrained grids such as constrained delaunay triangulation [9, 10]. Constrained grids are the grids that keep some initial given structure elements such as pre initialized curves or edges, surfaces and volumes. This is the way we are going to add faults and fractures in the mesh.

In the case of unstructured grids several approaches exist at the moment [11, 12, 13, 14, 15]. But all of them based on the algebraic methods. In common case it is hard for algebraic methods to guarantee such good characteristics of grid as smoothness and proper cell forms. Best numerical grids keep the similarity of forms and sizes of adjacent cells all over the domain. Methods based on differential equations can be very handful in for this purpose.

Such differential methods are very widely used in structured grid construction. Methods are based on numerical differential geometry and those lead to very natural adaptation of structured grids [16, 17, 18]. There are very much of such approaches of constructing structured adaptive grids [19, 20, 21, 22].

Namely, the approach we are going to use is solving the inverted Beltrami equation [19, 17]. This approach guarantee the property of smoothness for cell form and size changes since it is based on variational methods. The equation is taken by minimization of energy functional which is based on theory of constructing isometric coordinate system on the surface [16]. Thus, the approach is the best in terms of the physicality of the result grids.

3 Materials and methods

3.1 Unstructured grid construction

To construct unstructured grids, we used Delaunay triangulation and Voronoy diagram [6] since they create comparatively good grids for computations on the given set of points using control volume methods. Delaunay triangulation is the triangulation of the set of points in which all the triangles and points satisfy principle of Delaunay (figure 1A). This principle states that the triangles are not to contain other points from set inside of their circumcircles. The goal is to create such grids in common cases with initial structural limitations such as pre-defined edges that cannot be reconstructed.

To implement support of limitations we chose iterative method that allows adding new points to existing Delaunay triangulation. On figure 1 cases of adding new points inside the triangular cells and on the existing edge are demonstrated. Simple fragmentation of those cells may lead to appearance of cells that does not satisfy the principle of Delaunay. For such triangle and point we have to make flip operation, i.e. change diagonal in quadrilateral convex figure constructed on those 4 points (figure 1, E).

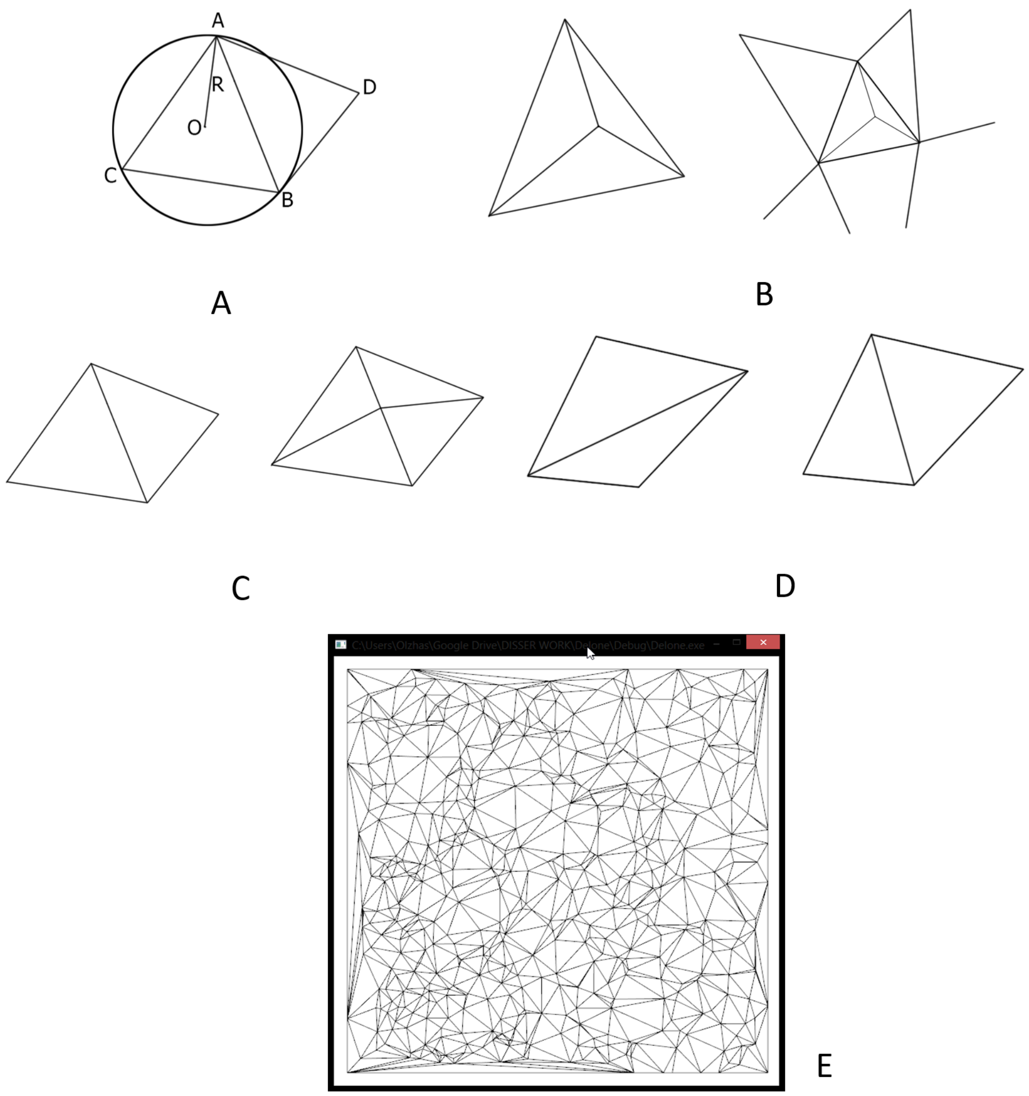

Figure 1 - Delaunay triangulation: A) Delaunay principle; B) Delaunay construction: adding new point in triangular cell; C) Delaunay construction: adding new point to existing edge; D) flip operation; E) demonstration of constructed triangulation on the random 100 points

Diagram of Voronoy is constructed using Delaunay triangulation by constructing central perpendicular segments for every triangle of Delaunay triangulation. Those segments connect mass centers of corresponding triangles. Such grid has many positive sides for computation using finite volume methods.

3.2 Adaptive structured grid construction

Structured grid adaptations are based mostly on solving differential elliptic equations. Consequently, they tend to smooth scattering of nodes of the grid. They find the mapping of some sample domain with common cartesian grid to the given physical area (figure 2, A). One of the most advanced in terms of adaptation is the method based on solving reversed Beltrami equation. The following equation is the reversed Beltrami equation that can be used to construct structured grids adaptive to gradients or values of scalar fields or to directions of vector field [19, 17].

$$\frac{\partial}{\partial s^j}(\sqrt{g^s}g_s^{jl}) = \sqrt{g^s}g_s^{im}\frac{\partial^2 s^l}{\partial\xi^i\partial\xi^m} \tag{1}$$

In the formula (1), repeating indexation means summation over those indexes on the one side of equality. S represents new grid coordinate system and ξ^i is initial grid's curvilinear coordinate system. Here $g_s^j l$ are contravariant tensor components and g^s is its determinant of the mapping shown in figure 2, A. Equation (1) is non-linear in such form and cannot be solved using standard elliptic equation solving methods, so to solve it we have to add time derivative. Thus, we convert it into parabolic equation and solve it by iterations. In each iteration we get new curvilinear grid which is little closer to the result adaptation than the previous one. Boundary conditions in those methods are taken by solution of the same problem on the lesser dimension. For 3D domain it is surface grid construction which in turn uses curve 1D grids as boundary conditions. The result grid constructed by described method shown in figure 2.

3.3 Proposed adaptive unstructured grid method

The unstructured grid construction method described above can construct it on any point set. So, the problem is initialization of the proper point set.

Our way to choose the point set is to use curvilinear adaptation provided by differential methods. The set is uniformly scattered on the sample domain, which is represented on the left side of figure 2, A. So, after mapping it represents uniformly scattered set with adaptation to the values of some scalar control function. Further this adapted set of points is used to construct the unstructured grid. Figures 3 and 4 demonstrates the results of the implementation of proposed algorithm. The points in figure 3 are chosen simply as the nodes of structured grid after adaptation. Since the sample cells are squares adaptive grid lines are still close to orthogonal. Therefore, in triangulation represented in figure 3, B, we can see that triangles are close to right triangles.

Figure 4 demonstrates unstructured grid constructed on the adaptive set of points. This set defined by mapping of regular triangulation on the sample field.

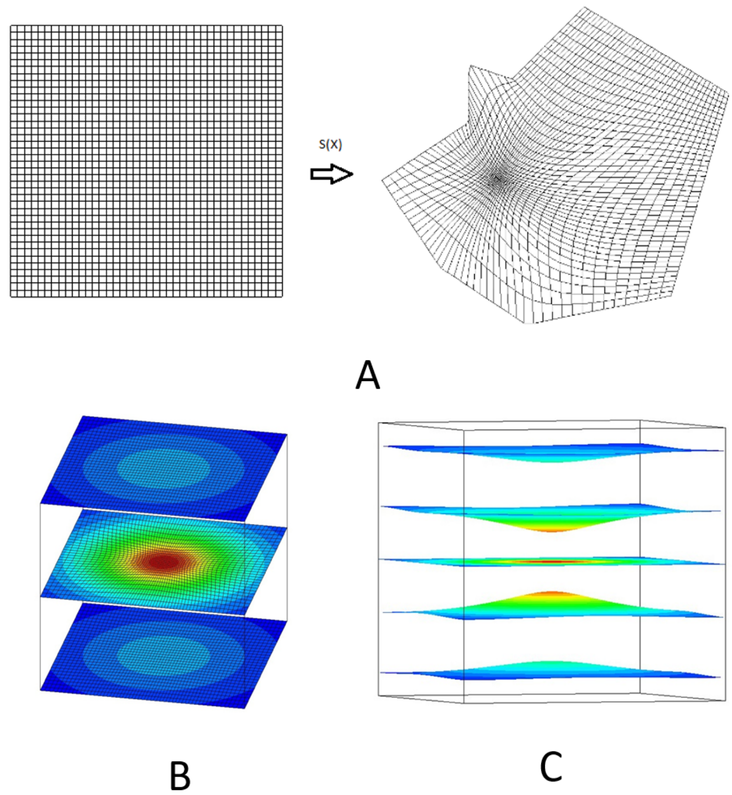

Figure 2 - Structured grid construction: A) mapping demonstration; B-C) using reversed Beltrami equation, control function is presented by colors

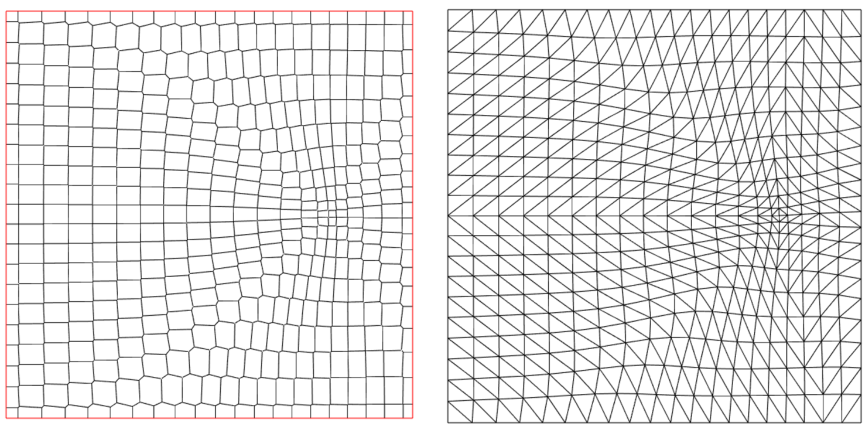

Figure 3 - Example of unstructured grid constructed using points set defined by nodes of adaptive structured grid: left – Voronoy diagram and right – Delaunay triangulation

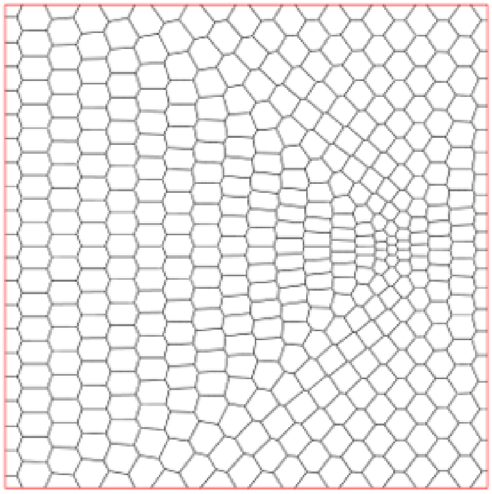

Figure 4 - Example of unstructured grid constructed using adaptive close regular points set

4 Results and discussion

In real industrial applications of physical simulation, the domain of physical process may have very complicated forms. They may have inner limitation structures, such as faults or fractures or very sophisticated boundary topology. In such cases it is very hard to use structured grids even with adaptation. Adaptive structured grids demand choosing sample domain for mapping close enough to physical one. Since in opposite case it is possible to generate prolongated cells of grid. This process is not automatized at all and it is the first serious drawback of the adaptive structured grids.

Complicated boundaries force researchers to make extremely fine grids near those boundaries in structured grids. Because the topology of the boundary has to became smoother in inner part of the domain. It leads redundant amount of fine parts and overall loss of optimization. In case when the domain has structural elements that put limitations for computational grid construction such as, for example, faults and fractures of porous media or some objects inside of continuous media, etc., unstructured grids also have benefits comparing structured grids. Those structural lines or surfaces can intersect in random order and make complicated non-structured topology. In such cases it is impossible for grid lines to trace the limitation lines. But in many cases, it is necessary to trace those lines as accurate as possible in numerical methods since the behaviour of the model along them are very critical to correctness of the solution.

Those advantages of unstructured grids fully preserved in our method since our result grid is unstructured grid. Only the choose of the sample domain for adaptive structured grid generation is still not automatized and have to be done manually before construction. However now it is not such limited as in construction of fully structured grid on the physical domain. Now the mapping must not map exactly to given boundaries. In general, it is enough to map to some area that contains whole physical domain. Researcher still have possibility to manually bind some boundaries or inner grid lines to boundaries or inner structural limitations of physical area correspondingly to get grids with proper tracing of such structural elements.

Adaptive structured grids in turn have main advantage that briefly can be stated as physicality of adaptation. Since we got adaptation on the base of solving differential equations that also used to describe the behaviour of physical simulations. Namely elliptic equations are used to implement diffusion processes and, therefore, to produce smoothly adaptive grids. This leads to smooth changes of such grid cell properties as size and elongation, i.e. how much the cell is squeezed in one dimension.

Existing unstructured grid adaptation techniques are based on using algebraic, geometry and graph algorithms. It is very unnatural and unconvenient to design those methods in such a way that they can guarantee the smoothness of such properties of the grid. Most of them does not guarantee that there are no leaps in size changes of adjacent cells. But the smoothness of size and forms of cells shows positive impact on the accuracy of the overall numerical method.

Unlike them differential methods based on elliptic equations guarantee such smoothness. It is due to fundamental property of elliptic equations to even the values of solution. Also, the method of solving reversed Beltrami equation is based on minimization of energy functional. It constructs the adaptive coordinate system in such way that grid cells are close to equal in case when the control metric is the metric of the surface itself.

Our method keeps that smoothness property of adaptive grid and transfer it to unstructured grids. Initial point set on sample domain is regular triangular grid nodes and its adaptation tries to keep those regularity. Due to that fact inner angles of cells are close to each other in the whole triangulation. Exceptions may occur if we need to add structural limitation lines that are not traced by structured grid lines because in such case initial point set has not any kind of relation to the predefined structural line or surface.

One significant drawback of adaptive structured grids is the process of using it with finite difference methods. Since the computational grid on physical domain is a mapping of some sample grid researchers must bring the expression to the correct form. Expressions are to be modified by substituting function to be found by its complicated mapped form and further implementation of all the derivations. Thus, researcher obtains complicated equation with Jacobians of the mapping and components of the metric tensor. Simple heat transfer equation is written in the following form

$$\begin{aligned}\frac{\partial u}{\partial t} = \nu \Bigg(& \frac{\partial}{\partial \xi^1}(\sqrt{g}g^{11}\frac{\partial u}{\partial \xi^1} + \sqrt{g}g^{12}\frac{\partial u}{\partial \xi^2} + \sqrt{g}g^{13}\frac{\partial u}{\partial \xi^3}) + \\ & \frac{\partial}{\partial \xi^2}(\sqrt{g}g^{21}\frac{\partial u}{\partial \xi^1} + \sqrt{g}g^{22}\frac{\partial u}{\partial \xi^2} + \sqrt{g}g^{23}\frac{\partial u}{\partial \xi^3}) + \\ & \frac{\partial}{\partial \xi^3}(\sqrt{g}g^{31}\frac{\partial u}{\partial \xi^1} + \sqrt{g}g^{32}\frac{\partial u}{\partial \xi^2} + \sqrt{g}g^{33}\frac{\partial u}{\partial \xi^3})\Bigg)\end{aligned} \tag{2}$$

This process has to be done manually for every equation in the model and yet has not any automatization. Solving the same equation with the finite volume method is much easier. Taking into account the fact that we have constructed Voronoy diagram and choose initial points as cell centers we can avoid non-orthogonal diffusion components in approximation. This approximation has not any differences from any other unstructured grid.

However, the most important reason to use adaptive structured grids is a possibility to use finite differences method with higher order approximation difference schemes. Proposed approach may be handy in situations when those schemes are not necessary.

5 Conclusion

The paper describes methods of unstructured grid construction based on differential methods. Differential equations are very good when it is necessary to create adaptive grids with smooth change of cell sizes and forms. Up to the moment such methods were used mostly for construction of adaptive structured grids. To transfer this property to unstructured grids we implemented standard grid construction algorithms with ability to construct grid on any given set of points. Further we choose the set of points that are going to be nodes of the Delaunay triangulation and centres of Voronoy diagram by solving boundary problem for reverse Beltrami equation. Solving the equation provides certain mapping of some sample grid to physical domain and we use that mapping to define the point set with adaptation.

Such approach gives us a list of advantages comparing raw adaptive structured grids. It is more effective and convenient to use in most cases except the case when it is important to use finite difference approximation schemes of higher order. Also, such method has good influence to adaptation of unstructured grid since differential elliptic methods have fundamental property to smoothen the solution.

6 Future work

This work is the first step of using differential methods for unstructured grid construction. At the moment it is simple sequential execution of two algorithms using the results of structured adaptive grid as an initialization point set to unstructured grid construction. Further work is going to be aimed to solving of the described differential equations by FEM or FVM methods for construction of unstructured grids.

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References

[1] Thompson, Joe F., B. K. Soni, and N. P. Weatherill. *Handbook of Grid Generation.* Boca Raton, FL: CRC Press, 1999.

[2] Shewchuk, J. R. "Unstructured mesh generation."In U. Naumann and O. Schenk, editors, *Combinatorial Scientific Computing.* , CRC Press, chapter 10 (2012):257–297.

[3] Lo, S. H. "A New Mesh Generation Scheme for Arbitrary Planar Domains." *International Journal for Numerical Methods in Engineering.* 21, no. 8 (1985): 1403-426. doi:10.1002/nme.1620210805.

[4] Peraire, J., J. Peir?, and K. Morgan. "Adaptive Remeshing for Three-dimensional Compressible Flow Computations."Journal of Computational Physics 101, no. 1 (1992): 229. doi:10.1016/0021-9991(92)90068-a.

[5] Shewchuk, J.R. "Tetrahedral mesh generation by Delaunay refinement." *Symp. on Comp. Geom.* (1998):86–95.

[6] Klein, Rolf, Franz Aurenhammer, and Der-Tsai Lee. *Voronoi Diagrams and Delaunay Triangulations.* New Jersey: World Scientific, 2013.

[7] Yerry, Mark, and Mark Shephard. "A Modified Quadtree Approach To Finite Element Mesh Generation." *IEEE Computer Graphics and Applications.* 3, no. 1 (1983): 39-46. doi:10.1109/mcg.1983.262997.

[8] Mitchell, Scott A., and Stephen A. Vavasis. "Quality Mesh Generation in Three Dimensions." *Proceedings of the Eighth Annual Symposium on Computational Geometry - SCG.* 92 (1992). doi:10.1145/142675.142720.

[9] Frederick, C. O., Y. C. Wong, and F. W. Edge. "Two-dimensional Automatic Mesh Generation for Structural Analysis."*International Journal for Numerical Methods in Engineering* 2, no. 1 (1970): 133-44. doi:10.1002/nme.1620020112.

[10] Der-Tsai Lee and Arthur K. Lin. "Generalized Delaunay Triangulations for Planar Graphs.„ *Discrete & Computational Geometry*, 1 (1986):201–217.

[11] Bronson, Jonathan R., Shankar P. Sastry, Joshua A. Levine, and Ross T. Whitaker. "Adaptive and Unstructured Mesh Cleaving." *Procedia Engineering.* 82 (2014). doi:10.1016/j.proeng.2014.10.389.

[12] Riemslagh, K., and E. Dick. "A multigrid method with unstructured adaptive grids for steady Euler equations." *Journal of Computational and Applied Mathematics* 67 (1996): 73-93.

[13] Vilsmeier, R., and D. H?nel. "Adaptive Methods on Unstructured Grids for Euler and Navier-Stokes Equations." *Computers & Fluids.* 22, no. 4-5 (1993): 485-99. doi:10.1016/0045-7930(93)90021-z.

[14] Bronson, Jonathan R., Joshua A. Levine, and Ross T. Whitaker. "Particle Systems for Adaptive, Isotropic Meshing of CAD Models." *Proceedings of the 19th International Meshing Roundtable.* (2010). doi:10.1007/978-3-642-15414-0_17.

[15] Mavriplis, D. J. "Unstructured Grid Techniques." *Annual Review of Fluid Mechanics.* 29, no. 1 (1997): 473-514. doi:10.1146/annurev.fluid.29.1.473.

[16] Vekua, I. N. *Generalized Analytic Functions.* Oxford: Pergamon Press, 1962.

[17] Lisejkin, V. D. *Grid Generation Methods.* Cham: Springer, 2017.

[18] Castillo, Jose E. *Mathematical Aspects of Numerical Grid Generation.* Philadelphia: SIAM, 1991.

[19] Glasser, A. H., V. D. Liseikin, and I. A. Kitaeva. "Specification of Monitor Metrics for Generating Vector Field-aligned Numerical Grids." *Russian Journal of Numerical Analysis and Mathematical Modelling.* 20, no. 5 (2005):439-461. doi:10.1515/156939805775186686..

[20] Godunov, S. K., A. V. Zabrodin, and M. Ja. Ivanov. *Chislennoe reshenie mnogomernyh zadach gazovoi dinamiki (Numerical solving of multidimensional problems in gas dynamics).* Moscow: Nauka, 1976.

[21] Khakimzyanov, G. S., and N. Yu. Shokina. "Equidistribution Method for the Construction of Adaptive Grids." *Russian Journal of Numerical Analysis and Mathematical Modelling* 14, no. 4 (1999):339-358. doi:10.1515/rnam.1999.14.4.339.

[22] Thompson, Joe F., Z. U. A. Warsi, and C. Wayne. Mastin. *Numerical Grid Generation: Foundations and Applications.* New York: North-Holland, 1985.