基于平衡颗粒法生成地质体复杂节理面网格的方法研究

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摘　要

宏观地质体中错综复杂的节理拓扑关系给节理面网格的划分带来了困难，进而制约了对含复杂节理地质体的力学效应研究。文章提出了一种利用颗粒生成节理面网格节点的方法——平衡颗粒法。该方法首先将复杂节理系统按照节理交线进行分割，而后通过节理面内颗粒的随机排布产生密实、微嵌入的颗粒系统，进而采用全量法计算颗粒间的接触力，同时引入指向节理面中心的牵引势函数,在粘性阻尼的控制下，通过显式迭代，逐渐实现接触力产生的斥力与势函数产生的引力之间的平衡。算例表明，基于平衡颗粒法产生的节理网格节点排布均匀，在节理交线处未出现奇异节点，表明了该方法的正确性。

Kratos Multi-Physics Framework for Large Unstructured Mesh Simulation in Gid pre and post Processor

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Abstract

Dealing with large simulation and creating a highly parallelizable code is a growing challenge. Develop a code for distributed memory machines(DMMs) can be very different form developing a serial code in term of algorithms and structure. Ideally for the well-parallelized software pre-pared for high performance, the problem solving capability depends on the available hardware resources. But in practice there are several technical details which reduce the scalability of the system and prevent the effective

use of such a software for large problems. In this work we describe a two combined tools to solve and visualize large scale problems: Kratos MutliPhysics [3] framework and GiD [2] pre and post processor.

GiD is a universal, adaptive and user-friendly pre and postprocessor for numerical simulations in science and engineering. It has been designed to cover all the common needs in the numerical simulations field from pre to post-processing: geometrical modeling, effective definition of analysis data, meshing, data transfer to analysis software, as well as the visualization of numerical results. Kratos Multi-Physics is an open source generic multi-disciplinary platform for solution of coupled problems consist of fluid, structure, thermal and electromagnetic fields. The parallelization of this framework is possible and can be prepared and migrated for high performance computing (HPC) with minimum modification and is performed with objective of enforcing the less possible changes to its different solver modules and encapsulate the changes as much as possible in its common kernel. This objective is achieved thanks to the Kratos design and also innovative way of dealing with data transfers for a multi-disciplinary code. The migration has been verified by a set of benchmarks which show very good scalability.

References

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Biomolecular Surface/Volume Meshing and Visualization for Mathematic

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Abstract

It is a challenging task to generate quality mesh which can be used for emerging mathematical modelings of biomolecular systems.
In the first part, I will present a robust method and software TMSmesh developed recently to generate manifold surface mesh for complex biomolecular surface. A Gaussian surface is used to represent molecular surface. The method computes the surface points by solving a nonlinear equation directly, polygonizes by connecting surface points through a trace technique, and finally outputs a triangulated mesh. To guarantee the generated mesh is a manifold mesh, it is necessary to divide the surface into into single-valued pieces along each x,y,z directions by tracing the extreme points along the fold curves on the surface. TMSmesh is shown be able to generate quality surface mesh for arbitrarily large molecule in PDB. Volume mesh can be generated based on the TMSmesh surface mesh by applying a third-part software such as Tetgen.
In the second part, I will present a visualization system MMV developed in our lab. MMV is also specifically designed for continuum modeling community, featured by its multifunction of visualization, modeling and analysis of biomolecule, mesh, and simulation data.

Tetrahedral Mesh Generation: An Introduction and the State of the Art

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WIAS

Abstract

In this talk, I will give an introduction of some fundamental topics in tetrahedral mesh generation, and a brief review of the state-of-the-art algorithms and techniques. I will then talk some algorithms which have both theoretical properties and practical values. Experimental results regarding the practical behaviors of these algorithms are presented.

几何、网格及可视化

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摘　要

首先介绍几何建模是网格划分和可视化的基础，归纳几何建模方法和我们的研究及应用。
其次，简单回顾网格划分方法，并介绍我们的研究及应用。
最后，简单总结可视化方法，并且介绍我们在标量场、矢量场和张量场可视化方面的研究及应用。

Fast Methods for Computing Centroidal Voronoi Tessellations

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Abstract

A Centroidal Voronoi Tessellation (CVT) is a Voronoi tessellation in which the generators are the centroids for each Voronoi region. CVTs have many applications to computer graphics, data compression, mesh generation, and optimal quantization etc. Lloyd's method, the most widely method used to generate CVT, converges very slowly for larger scale problems. Recently quasi-Newton methods using the Hessian of the energy associated as a preconditioner are developed to speed up the rate of convergence. In this work a graph Laplacian preconditioner and two-grid methods are used to further speed up quasi-Newton schemes. The proposed graph Laplacian is always symmetric, positive de_nite and easy to assemble, while the Hessian, in general, may not be positive de_nite nor easy to assemble. Therefore the graph Laplacian works as a better preconditioner than the Hessian that needs modi_cation to be used a preconditioner. The two-grid method can be used to generate a better initial guess in a coarse level and further speed up the convergence. Numerical tests show that our preconditioned quasi-Newton methods combined with a two-grid method converges fast and has nearly linear complexity.

支撑科学计算后处理的数据管理技术

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摘　要

目前，在科学计算后处理阶段提出了TB量级计算结果数据的高效存储和访问需求。报告针对并行数值模拟数据从产生到使用过程中所面临的数据组织、存储和检索问题，给出相应的数据管理技术解决方案，介绍在数据表示、数据索引、高层I/O软件库研制等方面所取得的研究进展，展示在惯约聚变、高功率微波、材料科学等领域所取得的应用效果，希望获得与同行的进一步交流。

面向 **TB** 量级时变数据集的并行可视分析

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摘　要

在科学与工程计算中，在数千上万核上，模拟的模型通常包含数亿网格单元，输出的时变总量通常达到 TB 量级。时变数据集由数百上千的单时刻数据集组成。单时刻数据集分布存储在数千上万个文件中，数据规模达到 GB 乃至十 GB 量级。针对以上应用需求，研制和发展了并行可视分析软件平台。该平台具有丰富的数据操作、分析、查询和可视化方法，并实现多种方法的耦合使用。目前该平台已应用于武器物理、激光聚变、全球气候变化、复杂电磁环境、材料科学、地质灾害和地下水资源监测等领域。实际应用表明，对于单时刻 GB 量级数据，在数十上百核上，可视分析交互响应时间可控制在数秒以内，基本满足交互分析需求。

A Novel Geometric Flow-Driven Approach for Quality Improvement of Segmented Tetrahedral Meshes

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Abstract

We present an efficient and novel geometric flow-driven method for mesh optimization of segmented tetrahedral meshes with non-manifold boundaries. It is composed of geometric optimization and topological transformation techniques, so that both location and topology of mesh vertices are optimized. Due to the complexity of non-manifold boundaries, we categorize the boundary vertices into three groups: surface vertices, curve vertices, and fixed vertices. Each group of boundary vertices is modified by different shape-preserving geometric flows to smooth and regularize boundary meshes. Meanwhile, all vertices are relocated by minimizing an energy functional which is relevant to quality measure of tetrahedra. In addition, face-swapping and edge-removal operations are employed to eliminate poorly-shaped elements. Finally, the performance of our method is compared with a state of art method, named Stellar, for a dozen single-component meshes. We obtain similar or even better results with much less running time. Meanwhile, we validate the presented method on several segmented multi-component tetrahedral meshes, and the results demonstrate that the mesh quality is improved significantly.

大数据时代科研数据可视化与分析的挑战

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摘　要

大数据近年来被广泛关注。科学计算手段的进步，超级计算中心产出前所未有的模拟数据，新的大科学装置也在产生巨大的数据；另一方面以Facebook,QQ 等为代表的社交网络的兴起，以及 Twitte、微博等社会媒体的迅速崛起，每天都会产生 TB/PB 级别的数据。但是拥有大量的数据并不等于获得相应数据的价值。只有能够有效理解数据，才能真正利用好大量的数据。复杂数据，例如流场的演化，微博的用户关系、庞杂的事件发展对发展相应的分析工具提出了新的挑战和要求。而近来，可视化和可视分析越来越得到重视，是理解大数据的一种重要手段，越来越广泛地被应用到科学、工程、商业和日常生活中。和其他分析手段不同，可视化利用人类视觉认知的高通量特点，通过图形的形式表现信息的内在规律及其传递、表达的过程，是人们理解复杂现象，诠释复杂数据的重要手段和途径。可视化与可视分析通过交互可视界面来进行分析、推理和决策；从海量、动态、不确定甚至相互冲突的数据中整合信息，获取对复杂情景的更深层的理解；可供人们检验已有预测，探索未知信息；同时提供快速、可检验、易理解的评估和更有效地交流手段。本次报告我们将介绍可视化如何帮助科学家分析复杂流场，探索地震事件极其发生的规律，理解观测微小生物对象，表现大都市交通的拥堵，发掘微博扩散传播的路线；我们将讨论和分析大数据可视化和可视分析的前沿挑战和最新进展，包括原位/移位分析技术、数据不确定性表达分析、数据可视清洗，协同可视分析，以及如何利用社区力量和众包开展可视分析等问题。