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ScienceDirect
Journal of Computational Physics 227 (2008) 6720–6726
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

Short Note

Nanoscale adaptive meshing for rapid STM imaging

Stéphane Bedwani [a,*], François Guibault [b], Alain Rochefort [a,*]

[a] Department of Engineering Physics and Regroupement québécois sur les matériaux de pointe (RQMP), École Polytechnique de Montréal, C.P. 6079, Succ. Centre-ville, Montréal, Québec, Canada H3C 3A7
[b] Department of Computer Engineering, École Polytechnique de Montréal, Montréal, Québec, Canada H3C 3A7

Received 31 March 2008; accepted 1 April 2008
Available online 15 April 2008

PACS: 07.05.Tp; 73.40.Gk; 02.60.Gf; 05.60.Gg

Keywords: Mesh adaptation; Scanning tunneling microscopy (STM); Delaunay triangulation; Computational imaging

1. Introduction

The numerical evaluation of individual tunnel currents (pixels) constitutes the bottleneck of fast scanning tunneling microscopy (STM) imaging. The number and the position of grid points where the current is punctually evaluated have to be judiciously chosen to reveal the most important contrasts. In this note, we present an adaptive meshing approach that significantly accelerates the computation time to produce STM images by reducing the number of pixels to evaluate without affecting the final image resolution. This method iteratively reveals the STM image by selecting new probing locations that improves the image quality at each step.

A straightforward method to compute a STM image is to send a high resolution square grid to a solver that will return a pixel color intensity for each node [1,2]. Since pixel calculation is the most time consuming step but is independent of the grid quality, redefining the surface discretization will reduce the amount of computed pixels and thus the time required to compute an image. This process is a step by step image analysis in which zones of interest, such as contrasts related to adsorbed molecules or structural defects, are identified. Contrarily to mesh modeling where one creates an optimized mesh from a high resolution solution, here we want to iteratively build an optimized mesh from a coarse and previous solution. A Delaunay triangulation has been used to efficiently generate optimized meshes from high resolution images [3], and a similar discretization scheme is used in the present work. During mesh generation, standard point insertion algorithms [4] are favored over methods that enable coarsening and smoothing operations [5], since displacing or removing already computed pixels will results in undesirable exclusion of already computed data.

* Corresponding authors. Tel./fax: +1 514 340 4711 (A. Rochefort).
E-mail addresses: stephane.bedwani@polymtl.ca (S. Bedwani), francois.guibault@polymtl.ca (F. Guibault), alain.rochefort@polymtl.ca (A. Rochefort).

doi:10.1016/j.jcp.2008.04.005

2. Methodology

Simulated STM images have particular characteristics that need to be considered while meshing. First, they are essentially made of smooth contrasts, i.e. the solution is noiseless and has no strong discontinuities. This allows efficient image analysis while using a first and second order differentiation approach of intensities. Second, the tunnel current calculation is independent of the surface location. This means that several currents can be computed at the same time on a parallel computer, and the current locations can be non-uniform.

The main steps of our adaptive algorithm are presented as follows. First, the surface of a molecular system is discretized using an initial unstructured mesh. Mesh construction uses a Delaunay triangulation, which is an efficient and well known meshing technique that can be easily implemented. The first adaptive cycle begins by computing a tunneling current at each node of the initial mesh. Then, the computed image intensities are rendered and analyzed to detect the edges from image contrast. Once the edge detection is complete, weights are assigned to the triangles to determine which ones need to be refined at their barycenter to improve image resolution. A new adaptive refinement cycle begins by computing the tunneling current at each new node of the mesh followed by another image analysis. The surface analysis and solving process is repeated until the target resolution is obtained. These image analysis steps of the adaptive algorithms represent less than 1% of the time consumed to evaluate a single pixel.

2.1. Initial mesh

As a first step before adaptation, an initial mesh must present the following characteristics to obtain an accurate adapted solution. First, mesh points must be distributed uniformly across the surface to prevent small contrasts from being ignored during the image analysis step. Second, mesh density can be increased in areas more susceptible to contain contrasts. An STM image is based on the electronic properties of the surface atoms rather then their position, but, while studying a molecular system, it is reasonable to put an emphasis on locations near the studied molecules. The initial resolution may also be significantly coarser then the final image resolution, which usually corresponds to the highest resolutions obtained experimentally ($\sim$0.2 Å). If the initial mesh is too coarse, the image analysis will omit to detect some areas of interest and the final solution will prove incomplete. A minimal mesh resolution is thus used, that is determined heuristically, based on a priori knowledge of typical feature sizes that must be detected.

2.2. Mesh analysis

On a continuous image, an important variation of the pixel intensities reveals the contrast locations by detecting its edges. On a typical grid image, a differential analysis is usually performed by applying bidimensional discrete differentiation operators. In image processing, these operators are represented by convolution masks applied on an image resulting in edges enhancement; Sobel and Prewitt filters are examples of a gradient operator. In our work, such operators cannot be directly applied on unstructured meshes since they only work on regular grids. Instead, we will approximate these operators using a quadratic regression method [6].

2.2.1. Quadratic fit (QF)

A nodal analysis of an unstructured mesh is possible by quadratically reconstructing a local function using QF over a patch, spanning a subregion of the mesh built as follows. First, a central node and all its surrounding nodes forming a ring of elements is added to the patch. Then, a second ring composed of the nearest elements surrounding the first ring is also included. Applying a least square regression on pixel intensities of a quadratic surface z

$$z(x,y) = a + bx + cy + dx^2 + exy + fy^2 \tag{1}$$

with constant coefficients a, b, c, d, e and f, over a patch of sampling points. These coefficients are obtained by minimizing a residual for a patch of n elements. The regression is optimal if the sampling points are uniformly distributed around the studied node, but remains precise even for skewed elements. During an adaptive cycle, a differential analysis is performed for each mesh point associated to a patch and its fitted surface.