Adaptive Algorithms for Real-Time STM Imaging

S. Bedwani[1], *F. Guibault*[2] *and A. Rochefort*[1]
Département de génie physique[1] *et informatique*[2]*, École Polytechnique de Montréal,*
et Réseau québécois sur les matériaux de pointes[1] *(RQMP)*
Montréal, Canada
Stephane.Bedwani@polymtl.ca

Our present understanding of electronic transport theories enables us to compute STM images of large and complex molecular systems such as carbon nanotubes or self-assemblies. The production of numerical STM images is generally limited to relatively small systems and needs substantial computational resources. Nevertheless, through the fast evolution of computer power, in conjunction with new parallel algorithmic strategies, the synthesis of real-time STM images now appears feasible. A rapid evaluation of STM images will allow both experimentalists and theoreticians to work on a common platform that will simplify the analysis of experimental data and favor exploration of new materials.

In order to produce real-time STM images, a two stage strategy is envisionned: the parallelization of tunneling current calculations (as STM image pixels), and the discretization of space where these currents are computed. For the current calculations, we have already successfully implemented a parallel approach using the extended Hückel formalism based on periodic systems. The present work focuses on the second stage, which is based on an iterative process involving adaptive algorithms. The 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. This significantly decreases the computational time to produce STM images by reducing the number of calculations to perform in a specific areas.

The main steps of our adaptive algorithm are described in Figure 1(a). First, the surface of a molecular system such as the one illustrated in Figure 1(b) is discretized using an initial mesh. This step is performed either by taking a uniform coarse square grid or by using the position of adsorbed atoms. Several tunneling currents are then computed simultaneously for all mesh points on a parallel computer. For maximum flexibility, the tunneling currents can be probed anywhere on the surface, and the generated images are analyzed on an unstructured mesh obtained from a Delaunay triangulation. To locate the zones of interest, solutions are analyzed by detecting the edges, based on image contrast. Typical edge detection algorithms apply a convolution filter on a grid image to approximate the Laplacian. Although this process cannot be performed on unstructured meshes, it is still possible to approximate the Laplacian with a quadratic fit[1]. This fitting method approximates the second derivative for each pixel by applying a least square regression of a quadratic surface over a small area around a specific pixel. The Laplacian of the fitted surface yields a simple value that is assigned to the surface point studied. Once the edge detection is complete, weights are assigned to the triangles to determine which points of the surface need to be adapted to improve the image resolution. This adaptive cycling is then repeated until the desired resolution is obtained.

A sequence of adapted meshes is shown in Figure 1(c) where the final adapted solution contains only 945 pixels but has an equivalent resolution to a square grid of 3600 pixels. In this particular case, the adapted image is generated almost four times faster then the typical grid image. In addition to the molecular adaptive mesher, we will present advances in the virtual STM project.

Reference:

[1] C. Manole, M.-G. Vallet, J. Dompierre, and F. Guibault, “Benchmarking Second Order Derivatives Recovery of a Piecewise Linear Scalar Field”, In *Proceedings of the 17th IMACS World Congress Scientific Computation, Applied Mathematics and Simulation*, (2005).

Figure:

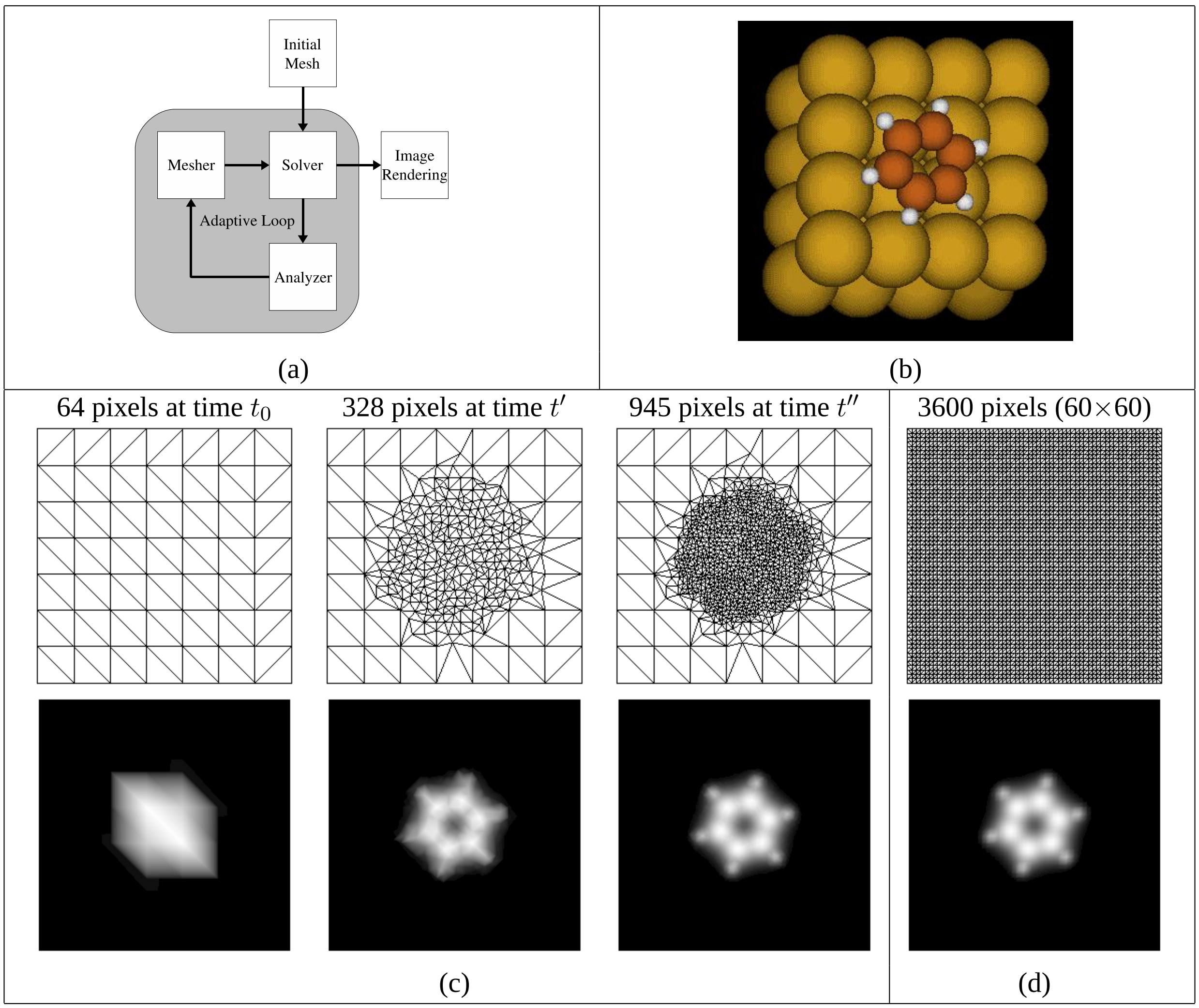

FIG. 1 – (a) Data flow of our adaptive molecular mesher; computations are performed on an initial mesh, then the surface is analyzed, and a new mesh is generated containing the next pixels to be solved. The surface analysis and solving process is repeated until the target resolution is obtained. (b) Benzene molecule adsorbed on Cu(100) surface is a simple example of an input system that can be used to generate numerical STM images. (c) Sequence of meshes and their ideal solution based on benzene’s Van der Walls surface for different stages of the adaptive algorithm; first image is an initial coarse grid, second is an intermediate unstructured mesh, and third is the final adapted solution. (d) Reference grid of 3600 pixels and a solution for comparison with the final adapted solution.