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Augmented Reality User Interface for Nanomanipulation using Atomic Force Microscopes

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Abstract. Models for a user interface for nanomanipulation using atomic force microscopes (AFM) are presented. Nano-scale 3D topography and force information sensed by the AFM-probe are blended with real time simulations and are fed back to the user. The sample surface is modeled with a spline-based geometry model, upon which a collision detection algorithm determines, whether and how the AFM-tip penetrates the surface. Based on these results, the induced surface deformations are simulated and 3D force feedback information is obtained. The simulated information is then blended in real time with the force measurements of the AFM in an augmented reality (AR) human machine interface, comprising a computer graphics environment and a haptic interface.

1. Introduction: AFM-based telemanipulation

Atomic force microscopes (AFM) are tactile imaging instruments with a resolution down to atomic scale. Offering highly precise positioning and force sensing, AFMs are employed not only for imaging, but also as teleoperated manipulators on the micro- and nanometer scale. The AFM-probe is controlled in a suitably scaled way by a haptic master device through which the user can feel the forces interacting between scanning tip and sample surface. Comprising also a 3D computer graphics environment, which displays a previously scanned image of the sample surface and the current position of the probe, these systems provide a highly intuitive way of interaction with objects on the nanometer scale. Yet, the design of AFMs puts two crucial constraints to these user interfaces:

- No visual feedback: Deformations induced by the AFM-probe cannot be seen as no imaging is possible while the tip is employed in teleoperation.
- No 3D force measurement: The force sensing of AFMs cannot resolve the force interacting between scanning tip and probed surface in three dimensions. As can be seen in figure 1, only two signals, $\Delta\theta$ for lateral forces in y-direction and $\Delta\alpha$ for both, frontal forces in x-direction and normal forces in z-direction, are measured.

These limitations are inherent in the design of AFMs and cannot be overcome easily. Visual feedback could be provided using hybrid approaches with e.g. SEM, but this again introduces new complications. Exact force feedback and position control could be gained by limiting the directions of movement to two dimensions, however if 3D feedback is desired, a new force sensing method is required [1].

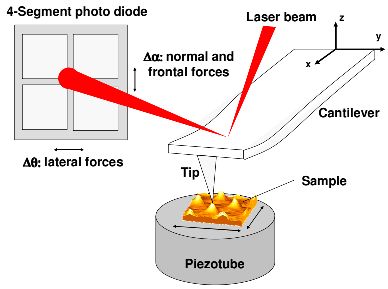

Fig. 1. AFM-force sensing: frontal and normal forces are measured in a coupled way.

2. Augmenting Measured with Modeled Information

In this study, models have been developed in order to simulate lacking information, i.e. surface deformations and 3D resolution of forces exerted on the tip. The following information is modeled as it cannot be determined from the AFM directly:

- Deformed shape of the sample surface in contact with the spherical scanning tip.
- Geometry of contact, respectively the normal direction of the contact between the arbitrarily shaped sample surface and the spherical AFM-tip.

Combining simulation results and measured information in real time, full 3D force feedback from the AFM-probe can be given to the user and otherwise invisible deformations can be visualized. Thus an augmented reality user interface for nanomanipulation, offering real 3D visual and haptic feedback can be provided to the user.

3. Spline-based Surface Model

The geometry of the sample surface is modeled as a spline, while the AFM-tip is assumed to be spherical [3]. A previously scanned image of the sample surface is first smoothened with a Gaussian low-pass filter to remove noise and then a bicubic B-Spline surface is fitted onto the data points. This yields a continuous, parametric representation **S**(u,v) of the sample surface. Intersections between the spline representing the sample surface and a sphere representing the AFM-tip can be detected by orthogonal projection of the tip's center onto the spline. Projecting a point **C** onto the spline surface **S**(u,v) corresponds to finding the shortest distance between **C** and a point of the spline. Solving this equation system for the two unknown u and v can be done using binary search [2] on the spline parameters u and v or the iterative Newton method, which was chosen by the authors.

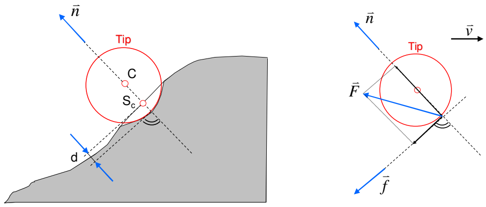

Fig. 2. Collision detection: Indentation depth and normal direction are obtained (left) and based on these, force directions can be derived (right).

The collision detection algorithm yields the point $\mathbf{S_C}$ closest to the center **C** of the spherical tip and also the normal direction $\vec{n}$ of the interaction between tip and surface and the indentation depth d, with which the tip penetrates the surface.

In order to visualize the deformation of the sample surface, the control points of the spline are repositioned in case of contact. With the indentation depth d known, the radius of contact can be obtained using Maugis' Dugdale Model [3]. Then all control points in the area of contact, i.e. which lie within the contact radius around the central line of contact, are projected onto the sphere representing the tip. This approach gives a visually good approximation for the shape of the deformed surface. This way, indentations of the sample surface can be visualized as well as adhesion effects, when the tip sticks to the sample.

4. Decoupling AFM Nano-Forces

Using the results of the collision detection, namely the indentation depth and the normal direction of the contact between tip and sample surface, the two force signals from the AFM can be decomposed into 3D.

For rectangular cross-sectioned cantilevers, the relation between forces exerted on the tip and the tip's deflection from its position at zero force can be treated analytically using the Bernoulli-Euler equation. Forces in lateral direction cause bending of the cantilever as well as torsion. The optical lever method however only measures angular twisting of the beam, which in case of torsion without bending is directly proportional to the exerted force. Therefore, wide and thin cantilevers, for which lateral bending can be neglected, are used. Lateral forces are then proportional to the torsion angle $\Delta\theta$ [4]:

$$\Delta\theta = cF_y \,, \qquad \textbf{(1)}$$

where c is a constant determined only by the beam's dimensions and its material parameters. Forces in normal and frontal direction both cause equally directed changes in angular orientation of the beam's end. Therefore their measurement obtained by the optical lever method, is coupled [1]. As the angular change $\Delta\alpha$ is very small, it can be approximated by the slope at the end of the beam $z'(l)=\tan(\alpha)$, which yields:

$$\Delta\alpha = \frac{l^2}{2EI}\left[F_z + \frac{2a}{l}F_x\right], \quad \textbf{(2)}$$

where a is tip height, l is the beam's length, E its Young Modulus and I its flexure momentum of inertia referred to the y-axis [4]. Neither F_x nor F_y can be determined directly from measured angular change. Yet with a simple geometric consideration, one more relation for the components of the overall force vector $\vec{F}$ can be obtained.

Considering figure 2, it is obvious that $\vec{F}$, consisting of a component normal to the surface and a friction component tangential to it, has to be in the plane defined by $\vec{n}$ and $\vec{f}$. The direction of the friction force is opposed to the tip movement represented by $\vec{v}$ and tangential to the surface at the contact point. Let $\vec{v}^T = (v_x, v_y, v_z)$ and e.g. $\vec{f}^T = (-v_x, -v_y, f_z)$, then:

$$\vec{f} \circ \vec{n} = 0 \Rightarrow f_z = \left(v_x n_x + v_y n_y\right) / n_z \quad \textbf{(3)}$$

Now, one can compute the vector $\vec{p} = (\vec{n} \times \vec{f})$, which is perpendicular to the plane the overall force is in. Knowing that $\vec{F}$ and $\vec{p}$ are perpendicular and thus $\vec{F} \circ \vec{p} = 0$, one can obtain the decoupled force components:

$$F_x = \left(\frac{p_y}{p_z}F_y + \frac{2EI\Delta\alpha}{l^2}\right) / \left(\frac{2a}{l} - \frac{p_x}{p_z}\right); \quad F_z = \left(\frac{p_y}{p_x}F_y + \frac{EI\Delta\alpha}{la}\right) / \left(\frac{l}{2a} - \frac{p_z}{p_x}\right).$$

Using the above equations, the force exerted on the tip can be resolved in three dimensions now using only the angular orientations ($\Delta\theta$, $\Delta\alpha$) measured by the AFM and the geometric information obtained from the collision detection algorithm.

5. Conclusion

By means of the introduced spline-based surface model, one can simulate and visualize the surface deformations caused by the AFM-tip in real time and resolve forces exerted on the tip and its deflection in 3D. This way, augmenting measured with modeled information, the quality of interaction with AFM-based nanomanipulation interfaces can be essentially improved concerning both visual and haptic feedback.

References:

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