Finding of the smallest enclosing cube

to improve molecular modeling

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Abstract

It is argued that by optimizing the orientation of a molecule in a cube can improve the efficiency of certain molecular modeling procedures.

INTRODUCTION

Molecular modeling involving large molecules frequently involves the overlay of a cubic grid around the molecule and the region around it. Examples for the use of such grid includes (but is not limited to) the calculation of the electrostatic energy of the solute with the surrounding dielectric (e.g., with the program Delphi [1,2]), calculation of volume elements in various proximal regions around solute atoms [3], calculating solvent density from a simulation trajectory. Since the total number of gridpoints is inversely proportional to the cube of the gridsize, reduction of the gridsize to increase numerical precision soon reaches computational limitations. However, by optimizing the orientation of the molecule to be modeled the enclosing cube can be reduced, resulting in a reduction of the gridsize without increasing the number of gridpoints.

METHOD

The orientational optimization has been implemented into the program Simulaid [4], using the simplex method for nonlinear optimization as described and programmed in Numerical Recipes [5]. For each orientation with Euler angles [6] (ϕ,θ,ψ) the program calculates the minimum and maximum of the x, y, and z coordinates, $x_{\min}$, $x_{\max}$, $y_{\min}$, $y_{\max}$, $z_{\min}$, $z_{\max}$. The corresponding enclosing cube's edge is $\max(x_{\max}-x_{\min}, y_{\max}-y_{\min}, z_{\max}-z_{\min})$ Thus the calculation of a single cube's size is linear in the number of atoms.

RESULT AND DISCUSSION

The program Simulaid already incorporates the optimization of orientation in various periodic cells and optimal centering [7]. Figure 1 (prepared by Simulaid on an SGI O2 workstation) shows the protein p53 in the orientation obtained from the PDB and after optimizing its orientation as described above. The edge of the original enclosing cube was 84.40 $\mathring{A}$, the edge of the optimized cube was 71.48 $\mathring{A}$, a reduction of 12.92 $\mathring{A}$. The minimization was performed from 10 different (randomly generated) orientations and half of the runs resulted in an edge shorter than 72 $\mathring{A}$.

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Figure caption.

1. The protein p53 before and after optimization with their smallest enclosing cube.