Folding@Home: New paradigms for molecular simulation

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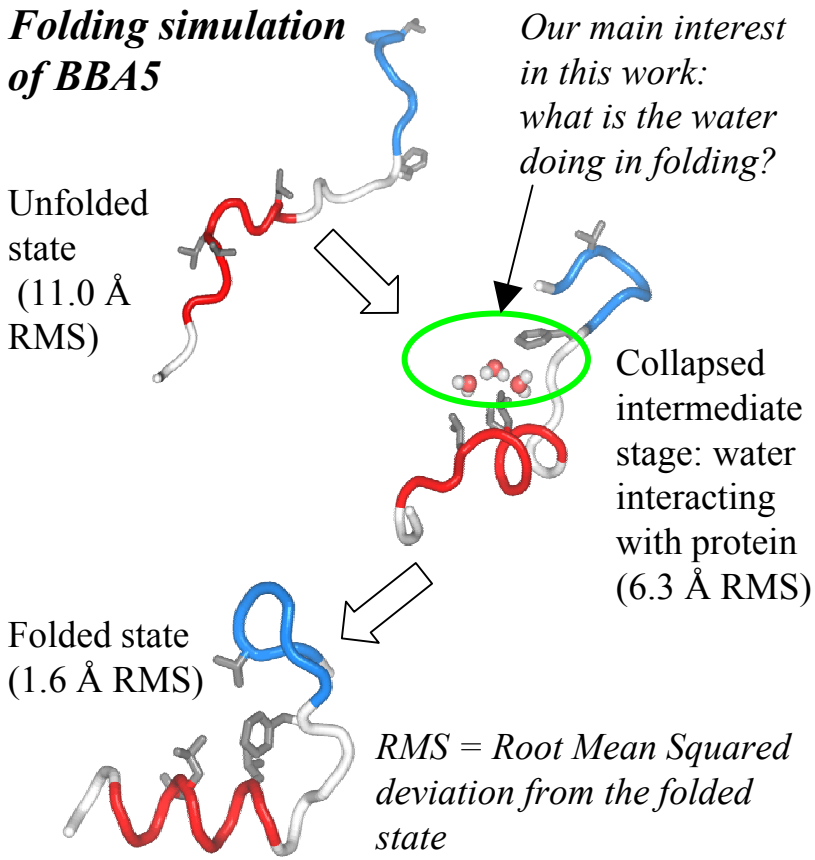
Before proteins can carry out their biological function, they must self-assemble, or "fold." Understanding folding is complicated by the nature of water. While water at first may seem like a simple liquid, it has many remarkable and complex properties. These properties, including the hydrophobic effect and hydrogen boding, can likely only be correctly understood with complex, "explicit" models for water. However, these models to date have been too complex to use in understanding long timescale behavior, such as folding. To overcome these timescales, a distributed computing project was created. This project, called "Folding@Home," now has the power of 100,000 PCs and this vast computing power combined with novel algorithms should allow one to simulate the role of water in protein folding for the first time.

Moreover, distributed computing allows for a novel "collaboration" with the general public. To help foster this active collaboration, we actively maintain a "chat room" for participants as well as many web resources to better understand proteins and protein folding. This directly connects with many of the broader impact criteria championed by NSF, including the goals of advancing discovery and understanding while promoting teaching (our education outreach sections of the web site), enhancing infrastructure for research and education (the distributed computing infrastructure itself), and broad dissemination to enhance scientific understanding (brought about and encouraged by the participation of people donating their time for the distributed computing project and their direct interest in the work being performed).



Y. M. Rhee, *et al*. *Proceedings of the National Academy of Science, USA* **101** 6456-6461 (2004)