New distrubuted computing mobile app lets phone conduct research while it charges

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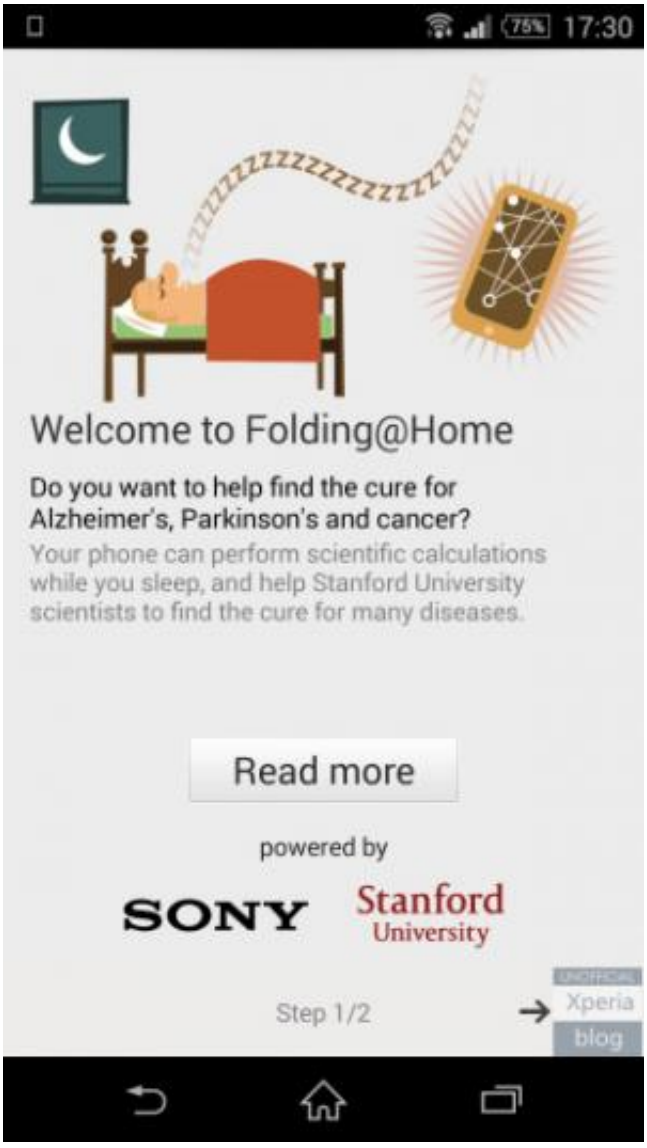

A new mobile app developed by Stanford Professor Vijay Pande and Sony Corp. allows smartphones to carry out protein-folding simulations while the phone is at rest and charging.

Your smartphone is already great for sending email, checking sports scores and sharing photos of your lunch. Now it can help battle cancer, Alzheimer's and other diseases, thanks to a new app developed by Stanford scientists and Sony.

The Folding@home mobile app, available today in the Google Play store, is an extension of the Folding@home distributed computing project launched by Vijay Pande, a professor of chemistry at Stanford, in collaboration with Sony in 2007. The new mobile app, Pande said, offers an opportunity to significantly expand on the original program, which has already simulated the structure of dozens of proteins and led to many important discoveries related to physiology and medicine.

"There are a ton of people with really powerful phones, and if we can use them efficiently, it sets the stage for something really great," said Pande, who also holds courtesy appointments in structural biology and computer science at Stanford.

Proteins are the molecules that make biology work, and understanding just how they do so requires a fine comprehension of their shape. They're produced as linear ribbons of molecules, and then snarl up like a ball of yarn, a process known as "folding."

The configuration of that snarl, though, is intensely critical to the protein 's ability to function properly. If a mutation or other malfunction shifts a few pieces slightly out of place, the protein's function will be impaired, it potentially won't work at all or, worse, it will work in a way that is harmful to the organism.

One of the best ways to study protein configurations is to predict the folding process using computers. Although it takes only milliseconds for

a protein to fold, the complexity of the process takes an incredible amount of computer power to simulate, requiring thousands of hours of computing time for even a supercomputer. To skirt this issue, in 2007 Pande and Sony launched the Folding@home project, tapping a distributed network of computer and Playstation 3 GPUs to simulate protein folding in their downtime.

The desktop program counts roughly 150,000 users and can provide full models of specific proteins – which are submitted for simulation at researchers' request – to scientists in weeks. As smartphones have become as powerful as desktops were just a few years ago, Pande and Sony began focusing on developing a way to take advantage of the rapidly growing population of mobile computers.

The mobile application is designed to run only when your phone is not in use, most likely as it charges while you sleep. Once you activate your phone, the application will shut down and seamlessly hand the simulation to another phone that is not in use, which Pande said should maximize the network's capacity.

At launch, Pande has chosen for the application to focus on simulating several configurations of a kinase protein involved in breast cancer. Scientists have found that individual breast cancer patients respond more favorably to different drugs, and they believe that this reaction might be due to individual differences in how this kinase is configured. Pande said that simulating a dozen or so possible configurations of the kinase, and then testing how these fit with a suite of drugs, could help identify better courses of treatment.

Doctors have a series of drugs to prescribe to patients, and they make their best diagnosis to choose which drug to give first. If Drug-A doesn't work, they move to Drug-B and so on. Depending on how advanced the cancer is, this process can take time that the patients simply don't have.

"We're going to learn a lot about the basic biophysics of kinases and their mutations, but we're hoping we can help doctors use genomic sequencing of tumors to say which drug should be given first," Pande said. "We want to help them pick a better Drug-A."

The kinase takes about 300,000 nanoseconds to fold, and a smartphone can simulate about one nanosecond per day, Pande said. If 10,000 phones work eight hours a day, the project could be complete in three months.

Once the enrolled smartphones simulate the proteins with enough specificity to be useful to scientists, the app will launch a new project, this one to investigate proteins associated with Alzheimer's disease. Eventually the app could host several projects, so that users could choose to contribute to a disease that is personally relevant.

For now, the beta version of the Folding@home app is compatible with Sony's Xperia Z series smartphones as well as the Xperia T3, T2 Ultra, M2 Aqua and C3, and is available for download from Google Play. Following the initial beta release, it will be made available for all smartphones running Android 4.4 and above later this year.

Provided by Stanford University

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