TITLE: Caring for our watershed using protein folding techniques

The concept of graphics processing relates to relaying information to a screen by running calculations through hyper-fast computer hardware. Computers are a valuable resource that lack the optimizations to be environmentally sustainable in their current state, however, if used correctly for running advanced calculations to progress an end goal, the outcome could not only be fundamentally efficient, but lead toward a world where we have a complete understanding of the foundations of all living things. My proposal uses my existing knowledge of enterprise computing to revolutionize the way a botnet could progress our societal development and improve existing functionality.

As a resident of Greeley Colorado the active watershed used by my residency is part of the Poudre watershed. The Poudre river supplies my city along with many of the surrounding cities, with clean drinking water. The safety of the watershed is taken as a priority, as early as 2012, fires erupted causing catastrophic damage to the watershed specifically. This was a call to action for the surrounding municipalities and thus multiple fire protection and more importantly, fire restoration committees. As the Poudre watershed was the primary source of water for smaller cities neighboring it, not to mention the highly dense agriculture, made the cleanup and reservation of the watershed. This series of events is the reason residents of Greeley have some of the best and most curated drinking water in the area.

One issue that is apparent in my watershed is that the quality of the drinking water is optimized for purity of its contents which makes perfect sense in an agricultural setting such as northern Colorado, however the problem lies in the systems we have in place to add and subtract mineralization to add taste and properties to the water. The science and rigorous testing that goes along with it, is bottle-necked by the means in which scientists can add minerals and other elements to drinking water. This is because the toxicity, oxidization, among other crucial factors plays a huge role in how the water tastes, but more importantly how these additives interact with the human body. This is a question water bottlers have been conjuring, and testing among the years. My proposal is this: From a scientific standpoint, how can we test minerals in water without risking adverse affects, From either human or animal testing? We can use computer algorithms that dynamically calculate equations that could be substituted for chemical composition after the fact, to test how human proteins interact with different variables on a 1:1 simulated level using enterprise level graphics processing modules, otherwise known as protein folding.

My solution to improve the local watershed is dynamic simulation techniques, efficiently optimized for improvement of human understanding for proteins and how they’re affected by different factors, by implementing a work schedule for school computers or computers in a similar academic environment, that allows them to be added to a network of like computers, to run simulations of protein dynamics during their usual “off” working hours. This solution has many advantages for an environment where computers are powered off for a majority of the day and night. The networks of computers setup alongside school resources such as web services and active directory login have been optimized for remote repairs, including that of the local computers making the implementation not only a feasibility, but a necessary change to help contribute good to a fast network built to help us understand the workings of everything that modern processor architectures can be tuned to contribute towards. Currently, the functions and

services used for other things inside the schools local network, are all that's needed to press a software package to every machine possible, given that machine is in a Wake on LAN state, with all the administration access granted and pre-configured to deny student access rights. Which in an academic environment, is always true. This method of acquiring data most likely goes strictly against the terms of use of the school computer resources, that being said with proper-intent and permission, My solution doesn't disallow any specific rights, nor causes any unnecessary damage to the machines running the simulations, so ideally the ambition is eccentric.

The Scope of my project is highly ambitious. With proper setup. It shouldn't be too hard to maintain the security of the location, manage folding computers, and with this information, decide the range of the project. Computer folding software is meant to be expandable, so running it on a single computer, and running it on a whole classroom of computers should in hindsight, be possible and easy to deploy. This can be done by using the tools already put in place by the network security experts that designed the local connections between "hubs" or sections of high traffic allocation areas of a network traffic. With this method of deployment, the relatively low powered, and hardly used physical desktop computers can be functionally turned into a botnet of local power accumulation for protein dynamics all while the computers would've been turned off or suspended otherwise. The scalability of this idea makes it easy for large contributions to scientific good, both locally, and in the future, developed to help the community, paid by taxes and maintained through the cloud, or on location, by the same person who manages the existing network. This means no extra cost needs to be associated with this type of software deployment making this method even more necessary for locations with large amounts of processing power that frequents a consistent working schedule. As for people that are needed we run into the first problem with this plan, in order to get all this software on all these computers, it's really easy. However, the control of what a local non-superuser can do is almost completely at the discretion of the network supervisor, or IT admin. So the duties of getting this unknown code in the schools eye, to the computers, so it can pursue its functionality of crunching numbers.

Proteins in living things, is a set of code, programmed into everything. The method in which we guess the effects of proteins to micro-bacteria, to Dirty water, to clean water, etc, to create an understanding of protein dynamics via software using the same mathematical equations mathematicians have found as constants in our universe. As an end goal to progress the technology, and work toward a greater good using government funding. I believe this to be a feasible idea because the premise of running calculations to improve human livability should be supported by the same system sought to educate human livability. And with no initial deposit or associated risk academic societies must understand not the current potential, but the future potential for such a system(s) in place. This is going to work because it contributes toward the ultimate power of comprehension among humans. Among the local water systems, CPU/GPU folding, future proofs world problems by decreasing the likelihood of a transmittable or obtainable body of infraction, that could be considered as world threatening. Considering our current and future political climate, the adoption of newer simulations has a vast slew of positives that span far beyond just the local watershed and could have even more adverse effects on communities with less prioritization with water rights and water management. The end

goal of this project and projects like it is to inspire academic institutes to donate computer power for global harmonization.

The projected scalability of this project is a main concern as with any network of compute power. The process a single computer goes through when running protein folding simulations should be predictable and static for expansion to a network, and the computers should keep their full functionality during working hours, this means a student who needs to use the computer should have no indication that the machine's status was affected, this means the computer should never store data on disk during this time. The software packages distributed should be extraordinarily lightweight and autonomous in functionality, as the end goal of this is to create an autonomous system using hardware that otherwise is powered off the entire night. Human understanding of protein dynamics will significantly improve my local watershed by providing data mining, and simulation capabilities for scientists specializing in water treatment and human science. With this idea I hope to inspire network administrators to encourage the use of folding and other process unit farming, by demonstrating the feasibility of running simulations on off hours, and explaining the usefulness of this data for scientific purposes on a global level.

Works Cited

Rice University. "New computer program accurately simulates protein folding dramatically faster than previous methods." ScienceDaily. ScienceDaily, 8 July 2010. <www.sciencedaily.com/releases/2010/07/100707112421.htm>.

Kuzmanic A;Bowman GR;Juarez-Jimenez J;Michel J;Gervasio FL;. (n.d.). Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Retrieved November 09, 2020, from https://pubmed.ncbi.nlm.nih.gov/32134250