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**Graphics processing units as tools to predict mechanisms of biological signaling pathway regulation** PATRICK MCCARTER, TIMOTHY ELSTON, MICHAL NAGIEK, HENRIK DOHLMAN, The University of North Carolina at Chapel Hill — Biochemical and genomic studies have revealed protein components of *S. cerevisiae* (yeast) signal transduction networks. These networks allow the transmission of extracellular signals to the cell nucleus through coordinated biochemical interactions, resulting in direct responses to specific external stimuli. The coordination and regulation mechanisms of proteins in these networks have not been fully characterized. Thus, in this work we develop systems of ordinary differential equations to characterize processes that regulate signaling pathways. We employ graphics processing units (GPUs) in high performance computing environments to search in parallel through substantially more comprehensive parameter sets than allowed by personal computers. As a result, we are able to parameterize larger models with experimental data, leading to an increase in our model prediction capabilities. Thus far these models have helped to identify specific mechanisms such as positive and negative feedback loops that control network protein activity. We ultimately believe that the use of GPUs in biochemical signal transduction pathway modeling will help to discern how regulation mechanisms allow cells to respond to multiple external stimuli.

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