Power Efficient In-Silico Drug Toxicity Prediction Through CUDA-Based Parallel Processing for Cardiac Cell Simulation

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***Abstract*—** **The persistent challenge of cardiovascular diseases as the leading cause of mortality worldwide necessitates innovative approaches in drug discovery to enhance public health. Traditional drug testing frequently relies on animal models, which often yield inconsistent results due to interspecies differences. This paper introduces an advanced computational method for predicting drug cardiotoxicity, using in-silico simulations. We address the computational inefficiencies by utilising CUDA-based parallel processing on graphics processing units (GPUs), including a modified simulation protocol for GPUs. Our approach significantly accelerates the single drug simulation process, achieving execution speeds of 13.4 times faster compared to existing central processing unit-based simulation. This speed boost saves predictively 183,960 Watt in processing 28 drugs of CiPA drug toxicity dataset. This efficiency not only propels drug discovery towards a more sustainable and rapid pipeline but also reduces reliance on animal testing, aligning with sustainability goals aimed at fostering innovation and infrastructure development, ensuring healthy lives, and promoting well-being at all ages.**

***Keywords*—** **Cardiotoxicity, in-silico, Graphics Processing Units, CUDA-Based Parallel Processing.**