**Enhancing the efficiency of animal-alternative in silico drug cardiotoxicity prediction through CUDA-based parallel processing**

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**Abstract**

(to be discussed after)

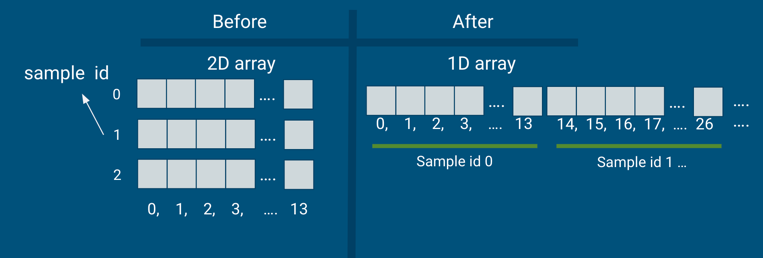


Figure 2. 1 Main difference in variable storing paradigm after CUDA-parallelisation

**1. Introduction**

Cardiovascular diseases (CVDs) remain the leading cause of mortality worldwide, highlighting the urgent need for efficient and reliable drug discovery pipelines. Current drug discovery pipelines face a significant challenge: the heavy reliance on animal testing. While this traditional approach has yielded important advancements, it raises significant ethical concerns regarding animal welfare. Additionally, animal models often exhibit limited ability to accurately mimic human physiology. This "species translation" issue can lead to misleading results, where drugs appear safe and effective in animals but fail to translate to human trials due to unforeseen safety risks or reduced efficacy.

In response to these limitations, in silico (computer-based) methods for drug cardiotoxicity prediction have emerged as promising alternatives. These methods offer a more ethical approach by eliminating the need for animal testing. Additionally, the potential for faster and more efficient drug development exists, as in silico models can potentially provide more accurate predictions of human drug safety and efficacy compared to animal models.

This research proposes a novel approach to address the computational bottleneck associated with complex in silico models by leveraging CUDA-based parallel processing on GPUs. This approach has the potential to significantly accelerate the execution of these models, making them more efficient and practical for real-world drug discovery applications. By effectively addressing these challenges, your proposed approach has the potential to significantly contribute to the development of a more efficient, ethical, and reliable drug discovery process**.**

**2. Method**

**a. Developing CUDA codes**

CUDA-based parallel programming is mainly using C/C++ style but in a different file format. Written in C style, the code is being saved using .cu and .cuh format, these are equivalent to .c and .h respectively. CUDA-based programming is able to accept C++ style object-oriented programming but in a very limited manner. One of the main limitation is the lacking the ease to use vector data type and multi-dimensional arrays in a live-shared (pooling) data manner. Vector data type required in the CPU version of the simulator to store simulation result as the result’s length might vary. Multi-dimensional array limitation require us to convert everything into a single dimentional array (flatten), and use a particular offset number such as in Figure 2.1.

**3. Results**

**4. Acknowledgements**

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**5. References**