Developing novel high performance computing approaches to cardiac simulation

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Multi-scale simulation of cardiac electrical activity is recognised as a fundamental approach in cardiac electrophysiology. However, a major obstacle often encountered in this field is the considerable computational power that is required to tackle physiologically and clinically relevant problems in practical time frames.

One way of tackling this type of computational challenge is to use massively parallel high performance computing systems, specifically *via* general purpose computing on graphics processing units (GPGPU). This methodology exploits the fact that a computationally demanding problem can be subdivided into many smaller ones that are solved simultaneously. This approach, however, introduces another rather complex technical challenge of how to develop, test, optimise, manage and validate cardiac simulation systems on massively parallel architectures.

In this study, we have developed a systematic approach to tackle this challenge resulting in six best practises for performing virtual organ level electrophysiological experiments:

1. Define experiment scope and tools formally
2. Estimate risks
3. Develop iteratively, with risk as the primary driver
4. Automate experiments
5. Continuously validate results
6. Organise experimental data effectively

Using the above methodology, we have built a virtual experimental environment consisting of more than 570,000 lines of highly optimised C++ code deployed on supercomputing infrastructure comprising 390 GPUs. The framework was used to simulate 80,000 heartbeats in 55 days, generating sufficient data for us to quantitatively analyse the molecular basis of ECG waveforms. The results achieved from this virtual experiment reproduced emergent clinical phenotypes from first principles and showed how epistasis can explain variable expressivity in disease. With the complexity of cardiac simulation scenarios set to continue to increase as more structural and biophysical details are incorporated into models, we suggest there is great potential for our approach to be used as a standard guideline in the cardiac simulation field.