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Agent based modeling of viral infections: an investigation across several spatio-temporal scales

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7. Discussion

In addition to the modeling challenges that we discussed in this thesis, there are technical limitations that also need to be overcome to succeed in an exhaustive replication of biological systems *in silico*. Achieving this grand challenge requires computing tools powerful enough to handle a multiscale model that simulates all or even parts of the spatio-temporal scales investigated so far. The discovery of new computing paradigms promises a realistic solution to the technical aspects of such multiscale models. New computing paradigms like general-purpose computing on graphics processing units (GPGPU) and cloud computing have provided solutions to maximize the utilization of currently available computing power. For example, GPGPU is extremely effective to perform fine-grained parallel computations such as simulating the individual molecular interactions (microscale) within a multiscale model of a virtual human. On the other hand cloud computing offers the infrastructure as a service (IaaS) model that provides resources on demand and scalability that would be essential to large-scale hierarchical computations. Simulating the immune response from molecular to cellular level within a single lymph node requires intensive computation, especially when an infection is taking place. A larger multiscale model that simulates all the lymph nodes in the human body interconnected by lymphatic vessels would greatly benefit from cloud computing since the simulation would not know in advance when and in which lymph node the infection will trigger the peak of computation. Thus using IaaS model would minimize the cost of running such a computationally intensive simulation, guarantee effective resource consumption and eventually make this multiscale simulation feasible.