

Mixed-Precision for solving large biological models

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In computational biology, agent-based models (ABM) are a computational modelling approach for complex living systems, enabling heterogeneity across agents. ABMs are often better aligned with data from real large systems [2]. However, the computational cost, which can increase supra-linearly with size, is a major challenge that limits applicability. In our work, we suggest to tackle this problem with the use of mixed-precision. Mixed-precision methods consist in using two or more numerical formats, usually floating point numbers [5], inside a single numerical method, to find a good trade-off between the accuracy and speed. These methods are developed in several fields that encounter similar dimensional computing problems such machine-learning [3], linear algebra [1] or meteorology [4].

Here, we consider an ABM of N heterogeneous agents described by a state variable in $X \in \mathbb{R}^{dN}$, where each agent is described by the d-dimensional sub-vector \mathbf{X}_i in \mathbb{R}^d , extracted from $\mathbf{X}_i = (X_{(i-1)d+1}, ..., X_{id})$. We assume that the dynamical dependence is split into two parts, an agentcentered term $F_i : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ and a term $G_{ij} : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ accounting for complex pairwise interactions, which are weighted by a vector $M_{ij} \in \mathbb{R}^d$. The state of each agent follows the nonlinear ODE :

$$\dot{\mathbf{X}}_i(t) = F_i(t, \mathbf{X}_i) + \sum_{j=1}^N M_{ij}(t, \mathbf{X}_i) \odot G_{ij}(t, \mathbf{X}_i, \mathbf{X}_j), \ i \in 1, ..., N,$$

where \odot is the Hadamard, or element-wise, product. We make no assumption on the form of G_{ij} , except that all the N agents can interact heterogeneously with each other. This leads to a right-hand side with a complexity in N^2 that is difficult to reduce.

We show that accuracy of numerical scheme is improved with the mixed-precision tuning as the system size increases. As the size of the population (N) increases, rounding errors coming from low precision terms are absorbed by the large number of interactions. This result is highlighted by a study exploring the parameters of three benchmarks. In addition, the complexity of non-linear functions used in modeling and the increasing size tend to increase the speed-up of low precision. This leads to an interesting gain in performance with a limited degradation in accuracy, particularly for interaction evaluations.

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