Mixed precision and local error in ordinary differential equations

Mouhamed AL-SAYED ALI, Inria - F-69603 Villeurbanne, France
Samuel BERNARD, Univ Lyon, UCBL, CNRS UMR5208, Inria, Institut Camille Jordan - F-69603 Villeurbanne, France

Arsène MARZORATI, INSA Lyon, CNRS UMR5208, Inria, Institut Camille Jordan - F-69603 Villeurbanne, France

Jonathan ROUZAUD-CORNABAS, Univ Lyon, INSA Lyon, Inria, CNRS, LIRIS UMR5205 - F-69603 Villeurbanne, France

In computational biology, many problems are modelled using individual-based or agent-based modelling. When expressed as ordinary differential equations (ODEs), these models lead to high-dimensional systems. The computational cost increases supra-linearly with the size of these systems. Accordingly, the solving of full-scale systems is intractable in terms of computational cost. Given that biological problems often have high empirical uncertainties, it could be possible to take advantage of the trade-off between computational speed and accuracy.
Mixed precision consists in using different levels of arithmetic precision within one computational task. Several fields already use this technique, such as geophysics [1] or machine learning [4]. Mixed precision methods have also attracted attention for problems involving differential equations [2].
Our study deals with a population of heterogeneous agents of size N, with $N \gg 1$, where each agent is described by a state variable $X_i \in \mathbb{R}^d$, which evolves according to an autonomous term $(F_i, i = 1, ..., N)$ and a term accounting for complex pairwise interactions $(G_{ij},\ i, j = 1, ..., N)$. The following system of equations describes the general framework. For $i = 1, ..., N$,

$$\dot{X}_i = F_i(X_i) + \frac{1}{N} \sum_{j=1}^{N} G_{ij}(X_i, X_j).$$

The evaluation of the N right-hand sides requires the sum of N nonlinear terms, leading to a $O(N^2)$ complexity. Reducing the precision used during the sum could accelerate the whole evaluation process by a considerable amount, as performed with iterative refinement solvers in [3].
To reduce the degradation of the global accuracy, mixing the precision inside the evaluations could allow minimizing the impact of the numerical error due to the insertion of low precision [5].
We performed tests on two benchmarks, and our results show that as the size of the system increases, the error introduced by low precision is absorbed by numerical compensation in high-dimensional systems. Moreover, the local error (in comparison with a double precision solver) measured by the solver is more robust to low tolerances in the case of mixed precision than a full low precision solver.

References

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Contact : arsene.marzorati@inria.fr