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Parallel stochastic simulation of cell-cell communication with spatially resolved reaction-diffusion kinetics

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Stochastic simulations are essential to the study of biological cells, yet there is no computational framework allowing for detailed spatial simulations of genetic regulatory network within large populations of cells.

We fill this gap by developing a parallel simulation framework capable of spatially resolved stochastic simulation of cell-cell signalling in multicellular systems. We use an operator-splitting method to decouple the internal reaction-diffusion kinetics from the interactions on the cells' boundaries and allow for efficient and horizontally scalable simulations of large numbers of interacting cells. Our framework is highly compatible with many existing methods and allows for hybrid simulation where both coarse and detailed models are considered at the same time. It is also greatly versatile and is deployable on various high performance computing platforms, such as clusters or clouds.

We use a small test model to study the convergence of our method as well as larger models to demonstrate weak scalability.

Our method demonstrate the feasibility of detailed stochastic simulations of large populations of interacting cells and is the first step toward more complete simulations including both detailed reaction-diffusion simulations and cell mechanics.

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