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ROBUST COMPUTATIONAL ALGORITHM FOR PARALLELIZED SIMULATIONS OF LIESEGANG PATTERNS

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Abstract. Liesegang patterns are unevenly spaced colored bands that can be obtained from the reaction of two specific substances, under diffusion-dominated conditions. The reactions involve the precipitation of one compound (most frequently salt crystals) which in turn forms the bands. This phenomenon has been studied more than a century ago but currently is getting increased interest since it can pose as an alternative for the bottom-up manufacturing of functional nano- and microstructures. In a previous work, a comprehensive numerical strategy for the numerical simulations of the dynamics of these processes able to solve the discontinuous nature of the phenomena, was presented. In such work, the well-posedness of the numerical formulation for the Liesegang pattern formation process was demonstrated. While the computational algorithm developed for OpenFOAM was accurately validated against literature, it was insufficient for simulating complex domains that demand higher computational power (like unstructured meshes), as it lacked compatibility with distributed memory platforms. The main characteristic of the strategy used to simulate the dynamics behind pattern formation is the communication of information in local domains around a specific area, to trigger or inhibit precipitation reactions. In this work, we propose a code framework that allows this original algorithm to be executed in parallel. OpenFOAM provides standardized communication tools, but to address the specific requirements of this phenomenon (such as determining whether reactions should be activated or inhibited at certain locations according to the model) the available primitives were leveraged and integrated to transmit information about the global domain's status. The developed framework was seamlessly integrated with the previous algorithm to simulate the pattern formation, and was tested against serial runs of the same scenarios, reducing greatly the simulation times but also allowing to obtain more precise results or enabling more complex domains, as far as denser meshes are allowed.

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