

PARALLEL NUMERICAL ALGORITHMS FOR NONSTATIONARY DIFFUSION-REACTION EQUATIONS ON GRAPHS

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We consider a reaction-diffusion parabolic problem on branched structures. The Hodgkin–Huxley reaction–diffusion equations are formulated on each edge of the graph. The problems are coupled due some conjugation conditions at branch points. On the branched structure (E, P) we consider a system of parabolic linear problems for a set of functions $\{u^k(x, t)\}$:

$$\begin{aligned} \frac{\partial u^k}{\partial t} &= \frac{\partial}{\partial x} \left(d^k \frac{\partial u^k}{\partial x} \right) - q^k u^k + f^k, \quad 0 < x < l_k, \quad k = 1, \dots, K, \\ 0 < d_0 &\leq d^k(x, t) \leq d_M, \quad q^k(x, t) \geq 0, \quad f^k = f^k(x, t). \end{aligned} \quad (1)$$

Here function $u^k(x, t)$ is defined on the edge e_k and the properties of each neuron can be different. At the first type branch points $p_j \in P_1$ the axial current is conserved:

$$\sum_{e_k \in N^+(p_j)} d^k \frac{\partial u^k}{\partial x} \Big|_{x=l_k} = \sum_{e_m \in N^-(p_j)} d^m \frac{\partial u^m}{\partial x} \Big|_{x=0}, \quad \forall p_j \in P_1. \quad (2)$$

At the branch points of the second type (corresponding to the soma in neuron models) the current flowing through the point $p_s \in P_2$ is a sum of currents coming in and leaving out through the local edges:

$$c \frac{\partial u_s}{\partial t} + q_s u_s = \sum_{e_m \in N^-(p_s)} d^m \frac{\partial u^m}{\partial x} \Big|_{x=0} - \sum_{e_k \in N^+(p_s)} d^k \frac{\partial u^k}{\partial x} \Big|_{x=l_k} + f_s, \quad \forall p_s \in P_2. \quad (3)$$

In this paper we investigate efficient parallel numerical algorithms for solution of such problems. We study three different types of finite-difference schemes. In order to decouple computations at each edge of the graph we consider two modifications of the implicit backward Euler scheme. In the predictor algorithm the values of the solution at branch points are computed by using the explicit approximation of the conservation equations. the predictor or predictor – corrector techniques. The stability analysis is done using the maximum principle method. In the predictor–corrector method in addition to the previous algorithm, the values of the solution at the branch points are recomputed by the implicit algorithm, when the discrete solution is obtained on each sub-domain. The stability of this algorithm is investigated only numerically.

Results of computational experiments are presented and the efficiency of the proposed parallel algorithms is investigated.