DIFFUSION SPLITTING METHOD FOR NON-STATIONARY DIFFUSION- ADVECTION-REACTION PROBLEMS

Roman Drebotiy

Ivan Franko National University of Lviv, Lviv, roman.drebotiy@lnu.edu.ua, roman.drebotiy@gmail.com

We propose certain semi-discrete splitting scheme for two-dimensional diffusion-advection-reaction initial-boundary value problem. Proposed approach admits further parallelizable full discretization with usage of the finite element method.

Denote by Ω a bounded domain with a Lipschitz boundary $\Gamma = \partial\Omega$. Let us define model parameters: diffusion $\mu = \text{const} > 0$, advection velocity $\vec{\beta} = (\beta_1(x), \beta_2(x))$, reaction speed $\sigma = \text{const} > 0$ and source term $f = f(x)$. Let us consider the following problem:

$$\begin{cases} \text{find function } u = u(x,t) : \bar{\Omega} \times [0,T] \to \mathbb{R} \text{ such that:} \\ u_t' - \mu\Delta u + \vec{\beta} \cdot \nabla u + \sigma u = f \quad \text{in } \Omega \times (0,T], \\ u(x,t) = 0, \quad (x,t) \in \Gamma \times [0,T], \ \Gamma := \partial\Omega \\ u(x,0) = u_0(x), \quad x \in \bar{\Omega}. \end{cases} \tag{1}$$

Problem (1) can be used in modeling of air pollution transfer over some geographical region. For this we should have known distribution of winds, or we can consider one-way coupled problem, where velocity $\vec{\beta}$ is a solution of Navier-Stokes equations.

We represent (1) in the corresponding variational formulation:

$$\begin{cases} \text{find } u \in L^2(0,T;V) \text{ such that:} \\ (u_t', v) + a(u,v) = \langle l, v \rangle \quad \forall v \in V, \end{cases} \tag{2}$$

where $V := H_0^1(\Omega)$ is a standard Sobolev space, $(w,q) := \int_\Omega wq dx$ and

$$\begin{cases} a(u,v) = \int\limits_\Omega (\mu \nabla u \cdot \nabla v + \vec{\beta} v \cdot \nabla u + \sigma u v) dx \quad \forall u, v \in V, \\ \langle l, v \rangle = \int\limits_\Omega f v dx \quad \forall v \in V. \end{cases} \tag{3}$$

Let us denote by $\vec{b}(x) := \vec{\beta} / \|\vec{\beta}\|$. Define vector field $\vec{\gamma}(x) = (\beta_2(x), -\beta_1(x))$ and corresponding normalized field $\vec{p} = \vec{\gamma} / \|\vec{\gamma}\|$. Let us define time step Δt and parameter $\theta \in (0,1)$. Let us denote by u_j (for integer j) an approximation to the function $u(x,t_j)$ at the time $t_j := j\Delta t$.

With certain restrictions on the vector $\vec{\beta}$, we introduce semi-discretization in time of the variational problem (2) with the following multi-step recurrent scheme:

$$\begin{cases} \text{given } u_j \in V, \text{ find } \dot{u}_{j+\frac{1}{4}}, u_{j+\frac{1}{2}}, \dot{u}_{j+\frac{3}{4}}, u_{j+1} \in V \text{ such that:} \\ (\dot{u}_{j+\frac{1}{4}}, v) + \theta\Delta t\, s(\dot{u}_{j+\frac{1}{4}}, v) = \langle l, v\rangle - s(u_j, v), \\ u_{j+\frac{1}{2}} = u_j + \Delta t\, \dot{u}_{j+\frac{1}{4}}, \\ (\dot{u}_{j+\frac{3}{4}}, v) + \theta\Delta t\, m(\dot{u}_{j+\frac{3}{4}}, v) = -m(u_{j+\frac{1}{2}}, v), \\ u_{j+1} = u_{j+\frac{1}{2}} + \Delta t\, \dot{u}_{j+\frac{3}{4}}, \\ \forall v \in V, \ \ 0 \le j \le T/\Delta t, \end{cases} \tag{4}$$

where

$$\begin{cases} s(u,v) := \int\limits_{\Omega} (\mu(\vec{b}\cdot\nabla u)(\vec{b}\cdot\nabla v) + v\vec{\beta}\cdot\nabla u + \sigma uv)dx, \\ m(u,v) := \int\limits_{\Omega} \mu(\vec{p}\cdot\nabla u)(\vec{p}\cdot\nabla v)dx. \end{cases} \tag{5}$$

We suppose that the problem data is quite regular, so all considered above variational problems have unique solutions.

We show, that we can build efficient parallelizable discretization procedure for finding the solution of each one of two variational subproblems of (4), in particular, with leveraging finite element method.

Proposed method uses typical approaches of building recurrent time integration schemes for variational problems [2]. The general idea of splitting the scheme and introducing intermediate fractional steps is known in the literature. For example, we can note famous Chorin's splitting method for Navier-Stokes equations [1].

1. *Chorin A.J.* Numerical Solution of the Navier-Stokes Equations, Mathematics of Computation, Vol. 22, No. 104 (Oct., 1968), pp. 745-762
2. *Trushevsky V.M., Shynkarenko H.A, Shcherbyna N.M.* Finite element method and artificial neural networks: theoretical aspects and application. – Lviv: Ivan Franko National University of Lviv, 2014, ISBN 978-617-10-0127-5 (in Ukrainian)