LadHyX Seminar – February 17, 14:00, – Room Jean Mandel (LMS)

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Simulating dislocation transport using a time-explicit Runge-Kutta discontinuous Galerkin finite element approach

In this talk, I will first present a very brief summary of more than 110 years of the development of dislocation theory, focusing mainly on the formulation of the dislocation transport initial boundary value problem. Then, the focus of this talk will be on the 3D numerical implementation of this problem using a time-explicit Runge–Kutta discontinuous Galerkin (RKDG) finite element scheme and some key results. The dislocation density transport equation, which lies at the core of this problem, is a first-order unsteady-state advection–reaction-type hyperbolic partial differential equation; the DG approach is well suited to solve such equations that lack any diffusion terms. The development of the RKDG scheme follows the method of lines approach. First, a space semi-discretization is performed using the DG approach with upwinding to obtain a system of ordinary differential equations in time. Then, time discretization is performed using explicit RK schemes to solve this system. The 3D numerical implementation of the RKDG scheme is performed for the first-order (forward Euler), second-order and third-order RK methods using the strong stability preserving approach. These implementations provide (quasi-)optimal convergence rates for smooth solutions. To demonstrate the predictive capabilities of the model, the following problems are solved: (i) Annihilation of two oppositely signed screw dislocations and (ii) the expansion of a polygonal dislocation loop. The RKDG scheme is able to resolve the shock generated during dislocation annihilation (a consequence of the first-order hyperbolic nature of the dislocation transport equation) without any spurious oscillations and predict the prismatic loop expansion with very low numerical diffusion. These results indicate that the proposed scheme is more robust and accurate in comparison to existing approaches based on the continuous Galerkin finite element method or the fast Fourier transform method.