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Lattice Boltzmann Method for Antiplane Shear with Non-Mesh Conforming Boundary Conditions

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Lattice Boltzmann methods [1] have been extended beyond their initial usage in transport problems, and can be used to solve a broader range of partial differential equations, e.g. the wave equation [2]. Thereby they can be utilized for fracture mechanics [3]. In the context of antiplane shear deformation we previously examined a stationary crack [4, 5] with a finite width. In this work we present two implementation strategies for non-mesh conforming boundary conditions, for which the bounding geometry does not need to adhere to the underlying lattice. This rectifies problems in modeling the crack. A numerical example shows the improvement compared to the previous results.

1 Lattice Boltzmann Method for Antiplane Shear Deformation

A linear elastic solid body is considered. The displacement $w(x, y, t)$ is regarded only in the x-y-plane, with out of plane loading applied along the z-axis. For such a system, Hooke's law together with a linear displacement-strain-relation reduces to a scalar 2D-wave equation, describing the time evolution of the antiplane shear deformation.

Lattice Boltzmann methods (LBM) use a statistical approach, where distribution functions f^α describe the state of the system, i.e. the state of the bodies deformation in this case. These are defined on a discretized lattice with spacing Δh, where each point is linked to its neighbors. The lattice velocities $\boldsymbol{c}^\alpha$ facilitate the exchange of information within one time step Δt. For $\alpha \in \{0, 1, 2, 3, 4\}$ this is called a D2Q5-scheme. An additional set of distribution functions f^α_{eq} per site describes a local equilibrium state. The time evolution of the distribution functions is given by relaxation towards these local equilibria, with relaxation time τ, via the lattice Boltzmann equation (LBE)

$$f^\alpha\left(\boldsymbol{x} + \boldsymbol{c}^\alpha \Delta t, t + \Delta t\right) = f^\alpha(\boldsymbol{x}, t) - \frac{1}{\tau}\left[f^\alpha(\boldsymbol{x}, t) - f^\alpha_{\text{eq}}(\boldsymbol{x}, t)\right]. \tag{1}$$

Which information is represented by the distribution functions depends on the model. For solving the wave equation, Guangwu Yan [2] proposed the interpretation as the velocity

$$\sum_\alpha f^\alpha = \frac{\partial}{\partial t} w = \dot{w}, \qquad \text{with} \quad w(\boldsymbol{x}, t + \Delta t) = w(\boldsymbol{x}, t) + \Delta t\, \dot{w}(\boldsymbol{x}, t + \Delta t). \tag{2}$$

The equilibrium distribution functions are defined as

$$f^0_{\text{eq}} = \frac{\partial w}{\partial t} - \frac{2\lambda w}{c^2} \quad \text{and} \quad f^\kappa_{\text{eq}} = \frac{\lambda w}{c^2} \quad \text{for } \kappa \in \{1, 2, 3, 4\}, \quad \text{with} \quad \lambda = \frac{c_s^2}{\Delta t}\left(\tau - \frac{1}{2}\right)^{-1} \tag{3}$$

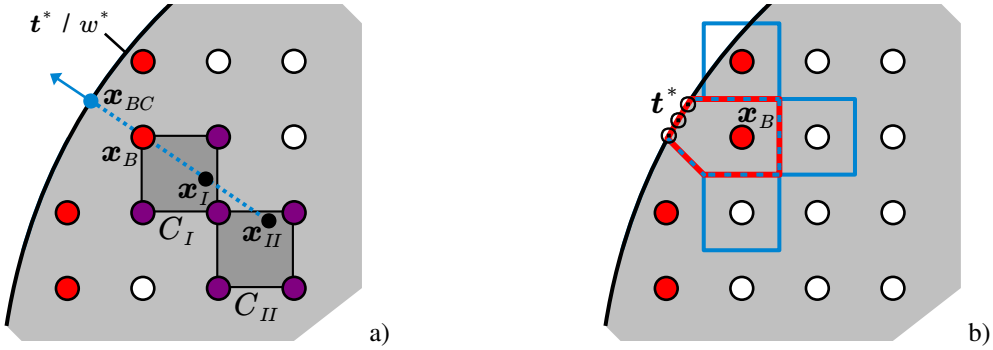

Fig. 1: Lattice configuration at a boundary. a) The macroscopic implementation approximates target values at $\boldsymbol{x}_B$ by interpolating in cells C_I, C_{II} containing $\boldsymbol{x}_I$, $\boldsymbol{x}_{II}$. b) The mesoscopic implementation considers the balance of momentum of a cell around $\boldsymbol{x}_B$.

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2 Non-Mesh Conforming Boundary Conditions

At a boundary some distribution functions are missing since the associated neighboring points lie beyond this boundary. Thus the prescribed boundary conditions need to be translated to these missing values of the distribution functions since the LBE (1) can otherwise not be used to update the distribution functions at boundary lattice points.

The *macroscopic* strategy utilizes interpolation to set target values. For a given boundary lattice point $\boldsymbol{x}_B$ the closest point on the boundary $\boldsymbol{x}_{BC}$ is identified. Along a line through $\boldsymbol{x}_B$ and $\boldsymbol{x}_{BC}$, as well as additional points in the interior, the displacement w_B is approximated by a second order polynomial, see Fig. 1 a). With proper constraints, either for Dirichlet or Neumann type boundary conditions, this leads to a linear system of equations $\boldsymbol{S}\boldsymbol{w}_B(t+\Delta t) = \boldsymbol{R}(t+\Delta t)$, that can be solved for the missing values. Since the interpolation regarding any $\boldsymbol{x}_B$ can involve other points along the boundary, this is a global system for all boundary lattice points. Now each of the n_{miss} missing distribution function at $\boldsymbol{x}_B$ is set to an the same value

$$f^{\alpha}(\boldsymbol{x}_B, t+\Delta t) = \frac{1}{n_{\text{miss}}}\left[\frac{w(\boldsymbol{x}_B, t+\Delta t) - w(\boldsymbol{x}_B, t)}{\Delta t} - \sum_{\beta\in\mathcal{F}_{\boldsymbol{x}_B}} f^{\beta}(\boldsymbol{x}_B, t+\Delta t)\right], \quad \forall\alpha\notin\mathcal{F}_{\boldsymbol{x}_B}, \tag{4}$$

where $\mathcal{F}_{\boldsymbol{x}_B}$ represents the known distribution functions from interior neighbors.

The *mesoscopic* implementation is based on cells surrounding a boundary lattice point $\boldsymbol{x}_B$, see Fig. 1 b), but only works for Neumann type boundary conditions. For such a cell the balance of momentum of one time step can be expressed using a finite difference as

$$\rho V_C \frac{\dot{w}(\boldsymbol{x}_B, t+\Delta t) - \dot{w}(\boldsymbol{x}_B, t)}{\Delta t} = T_C^{\text{ext}} + T_C^{\text{int}}. \tag{5}$$

Herein T_C describes the total traction for both the external boundary, which is given by the boundary condition, and the internal boundaries shared with neighboring cells. By identifying the contributions of distribution functions that are already known, the missing values can each be set to

$$f^{\alpha}(\boldsymbol{x}_B, t+\Delta t) = \frac{1}{n_{\text{miss}}}\left[\frac{T_C^{\text{ext}}\Delta t}{\rho V_C} + \dot{w}(\boldsymbol{x}_B, t) - f^{0}(\boldsymbol{x}_B, t+\Delta t) - \sum_{\beta\neq 0,\beta\in\mathcal{F}_{\boldsymbol{x}_B}} f^{\beta}(\boldsymbol{x}_B, t)\right], \quad \forall\alpha\notin\mathcal{F}_{\boldsymbol{x}_B} \tag{6}$$

Fig. 2 shows results for the numerical example of a stationary crack, as described in [5]. The stress intensity factor (SIF) is evaluated close to the crack tip at three distances. Fig. 2 b) compares both implementations presented here directly to previous results [5] of mesh conforming implementations and additionally to the finite element method (FEM). With these non-mesh conforming boundary conditions, the SIF is overall closer to the analytical solution, but still not as close as the FEM.

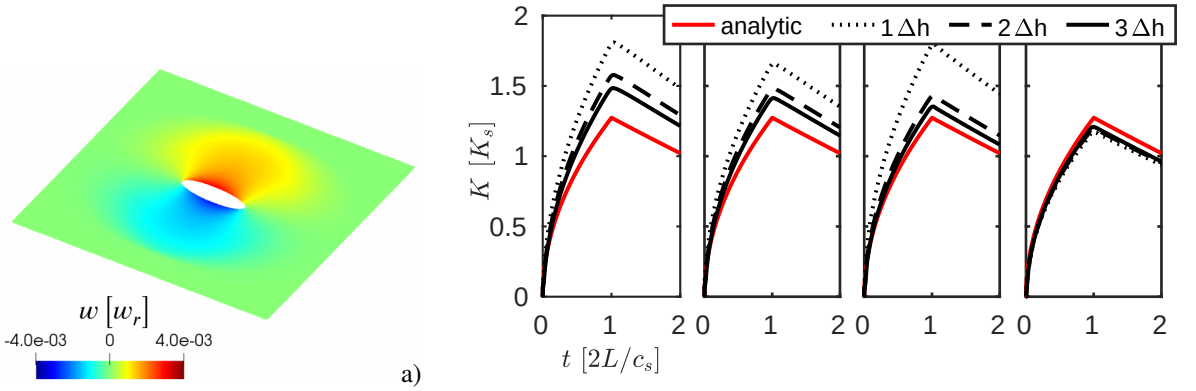

Fig. 2: The example of a stationary crack. a) A contour plot at $t = 1$, corresponding to the peak of the SIF. b) SIF with respect to time for different computational models. left to right: mesh conforming model, macroscopic, mesoscopic non-mesh conforming model, FEM.

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