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Efficient Flexible Boundary Conditions for Long Dislocations

M. Hodapp[1,2,*]

[1] *Skolkovo Institute of Science and Technology (Skoltech), Center for Energy Science and Technology, Moscow, Russia.*
[2] *Materials Center Leoben Forschung GmbH (MCL), Austria.*

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Abstract. We present a novel efficient implementation of the flexible boundary condition (FBC) method, initially proposed by Sinclair et al., for large single-periodic problems. Efficiency is primarily achieved by constructing a hierarchical matrix ($\mathscr{H}$-matrix) representation of the periodic Green matrix, reducing the complexity for updating the boundary conditions of the atomistic problem from quadratic to almost linear in the number of pad atoms. In addition, our implementation is supported by various other tools from numerical analysis, such as a residual-based transformation of the boundary conditions to accelerate the convergence. We assess the method for a comprehensive set of examples, relevant for predicting mechanical properties, such as yield strength or ductility, including dislocation bow-out, dislocation-precipitate interaction, and dislocation cross-slip. The main result of our analysis is that the FBC method is robust, easy-to-use, and up to two orders of magnitude more efficient than the current state-of-the-art method for this class of problems, the periodic array of dislocations (PAD) method, in terms of the required number of per-atom force computations when both methods give similar accuracy. This opens new prospects for large-scale atomistic simulations — without having to worry about spurious image effects that plague classical boundary conditions.

AMS subject classifications: 65N55, 70C20, 65N80

Key words: Atomistic/continuum coupling, flexible boundary conditions, local/global coupling, lattice Green functions, hierarchical matrices, dislocations.

1 Introduction

The advancements in hard- and software technology during the past decades have shifted the field of materials science towards a computer-assisted discipline making use of, in particular, atomistic simulations. Atomistic simulations can be used to study the nucleation, motion, and interaction of crystalline defects, e.g., vacancies, dislocations, grain

*Corresponding author. *Email address:* maxludwig.hodapp@mcl.at (M. Hodapp)

boundaries, voids, or cracks. In general, the goal of such studies is then to relate the behavior of those defects to macroscopic mechanical properties, e.g., yield strength, ductility, etc.

One major class of defects are line defects: the *dislocations*. It is well-understood that dislocations are the main carrier of plasticity in metals and their behavior is therefore intrinsically tied to any of the underlying strengthening and hardening mechanisms for this class of materials [5]. A representative behavior of long dislocations on the atomic-scale can be simulated with the periodic array of dislocations (PAD) method [18,45], where the periodic length in the dislocation line direction defines the intrinsic material length scale via the spacing of, e.g., obstacles (precipitates, voids, etc.). In addition to periodic boundary conditions in the dislocation line direction, the PAD method uses periodic boundary conditions in the dislocation glide direction and free surfaces in the direction normal to the glide plane. However, this particular choice of boundary conditions can introduce large image stresses, with spurious effects on the dislocation motion, as demonstrated by Szajewski and Curtin [61]. In particular, Szajewski and Curtin [61] have shown that, for a dislocation bowing around periodic obstacles, *all* side lengths of the simulation cell must be increased *equally* when varying the periodic length — but keeping the maximum bow-out constant — in order to maintain comparable accuracy in the final position of the dislocation. This implies that the PAD method scales cubically with the number of atoms which is very inefficient. To reduce this computational burden, conventional atomistic/continuum (A/C) coupling methods (e.g., [17, 22, 34–36, 44, 54, 62, 67, 68]) can be used to restrict atomistic resolution to some small part around the dislocation core, but scaling the side lengths of the computational domain with the periodic length is still required.

A natural approach that avoids the scaling issue of PAD boundary conditions is to use A/C coupling methods with *semi-infinite* continuum domains using boundary element methods (BEMs) [19, 28, 31, 39, 40]. To solve the coupled problem, Li [39, 40] further proposed an alternating Schwarz method which iterates between the atomistic problem and the BEM. A potentially more efficient method was developed by Hodapp et al. [28, 31] who proposed a monolithic Newton-GMRes solver with Hessian stabilization. However, the latter method is very difficult to parallelize and to integrate into existing molecular dynamics codes. The latter is a major concern since developers of A/C coupling methods are rarely users of their own codes which is likely the reason why many interesting approaches have been left unnoticed.

For coupling multiple codes, a much more convenient choice are domain decomposition methods, notably, in the field of A/C coupling, the *flexible boundary condition (FBC) method*, originally developed by Sinclair and coworkers in the 1970s [55–57], and newer related variants thereof [23,69] (another related method, independently developed specifically for contact problems, is "Green function molecular dynamics"; see, e.g., [14, 43]). However, an analysis of the FBC method has been developed only recently by Ehrlacher et al. [21] and Hodapp [29] who demonstrated its excellent convergence properties. In particular, Hodapp [29] showed that the FBC method can essentially be considered as