Coupling of continuum and particle models

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Abstract

In this report, we discuss the alternating Schwarz method as the classical domain decomposition method for solving partial differential equations, which we then use to couple particle and continuum models.

1 Introduction

Recently, many coupling methods have been developed in purpose of reducing the computational cost of simulations in molecular statics and molecular dynamics. Very often, full particle models are not efficient or even not feasible because of the large number of particles involved. On the other hand, the continuum models are computationally efficient compared to the particle ones, but not sufficiently accurate. A possible alternative is to use a particle model in the regions where continuum does not hold and to treat the rest of the regions by classical continuum theories. Hence, coupled models are employed, where the material domain is decomposed into particle and continuum subdomains. Usually, particle models are used only on small, strategically chosen subdomains where some irregularities are expected, and most of the body is modeled using a numerical approximation to continuum models such as the finite element method. The goal of such coupled methods is to be able to reproduce the results of fully particle models at a reduced computational cost.

There are many different approaches to couple particle to continuum models, but in general, little mathematical analysis exists for the majority of them, see for example the review paper [1]. In this paper they are roughly divided into energy and force-based methods. The alternative approach based on the classical alternating Schwarz method is omitted there as it can not be placed in either of these categories. However, the atomistic-to-continuum coupling problem is similar to the classical continuum-to-continuum domain decomposition problem. Exploiting the particular continuum-to-continuum domain decomposition method known as alternating Schwarz, in the atomistic-to-continuum context, is already been done to some extent, see for example [2] and [3]. However, there this approach has been used in very particular model examples, and very little error and convergence analysis exists.

Something more on the convergence analysis in the static case has been done in [4]. There, the authors explore similarities of atomistic-to-continuum coupling to the classical alternating Schwarz and give an estimation for the error along with the supporting numerical results in the one-dimensional case. Here, we discuss the algorithm proposed in [4] and present more thorough correlation of these two problems. In particular, we will point out what is needed to be done in order to show convergence of alternating Schwartz in an particle-to-continuum context. Moreover, we will extend what has been done in [4] to the non-matching grid case in order to make simulations faster. The coarser finite element grid will be coupled with the finer particle lattice, under the assumption that the particle model is used in the regions where some irregularities are expected so they could be captured with more care.

2 Schwarz formulation of domain decomposition method

Domain decomposition methods are used for solving partial differential equations in a divide and conquer manner. The computational domain is divided into subdomains with or without overlap, and then the
problem is solved on each of these subdomains by introducing some transmission conditions at subdomain interfaces. The Schwarz alternating method is one of the domain decomposition methods which is used in the case of overlapping subdomains. Here, we will focus on this particular method when domain of the elliptic equation is divided into two overlapping subdomains.

We consider the following second-order, self-adjoint, coercive elliptic equation with given Dirichlet boundary condition

\[ Lu \equiv -\nabla \cdot (a(x)\nabla u) = f(x), \quad \text{in } \Omega \subset \mathbb{R}^n \]
\[ u = 0, \quad \text{on } \partial \Omega. \]  \tag{2.1}

We are particularly interested in the numerical solution of (2.1) by finite elements. The discretization will result into a large, sparse, symmetric and positive definite linear system of equations. We start here by giving the weak formulation of (2.1), which is obtained by multiplying it by a test function \( v(x) \) with zero boundary value and integrating the resulting expression by parts over \( \Omega \). In the weak problem, we are seeking \( u \in H^1_0(\Omega) \) which satisfies the following

\[ a(u, v) = (f, v), \quad \forall v \in H^1_0(\Omega), \quad \text{where} \]
\[ a(u, v) = \int_{\Omega} a(x) \nabla u \cdot \nabla v \, dx, \quad (f, v) = \int_{\Omega} f v \, dx, \]
\[ H^1_0(\Omega) = \{ v \in H^1(\Omega) : v = 0, \quad \text{on } \partial \Omega \}, \quad H^1(\Omega) = \{ v \in L^2(\Omega) : \|u\|_{1,\Omega} < \infty \} \]
\[ \|u\|_{1,\Omega}^2 = \int_{\Omega} (v^2 + |\nabla v|^2) \, dx. \]

Now, a finite element discretization of (2.1) is obtained by Galerkin approximation of (2.2). Denote by \( \tau_h(\Omega) \) a triangulation with elements of size \( h \) and by \( V_h \) the space of continuous piecewise linear finite element functions on \( \tau_h(\Omega) \). If \( \{\phi_1, \ldots, \phi_n\} \) forms a basis for \( V_h \cap H^1_0(\Omega) \), then the finite element discretization of (2.2) yields the following linear system

\[ Au = f, \]  \tag{2.3}

where \( A_{ij} = a(\phi_i, \phi_j) \) for \( 1 \leq i, j \leq n \) and \( f_i = (f, \phi_i) \) for \( 1 \leq i \leq n \).

Instead of solving (2.1) on the whole domain \( \Omega \) at once, we will solve an equivalent problem which includes coupled system of partial differential equations defined on an overlapping decomposition of \( \Omega \). We say for two open subregions \( \Omega_i \subset \Omega, \quad i = 1, 2 \), that they form an overlapping decomposition of \( \Omega \) if \( \Omega_1 \cup \Omega_2 = \Omega \) and \( \Omega_1 \cap \Omega_2 \neq \emptyset \). The interior segments of the boundaries of these subdomains are denoted by \( \Gamma_i = \partial \Omega_i \cap \Omega \). This is shown in Figure 1.

![Figure 1: The overlapping decomposition of domain Ω consists of {Ω₁, Ω₂}](image)

To derive the coupled system for (2.1), let \( u(x) \) be a smooth solution of (2.1) and define \( w_i(x) = u(x) \) on \( \Omega_i, \quad i = 1, 2 \). Then by construction \( Lu = f \) in \( \Omega_i \), and the continuity of \( u \) will give matching of \( w_1 \) and \( w_2 \) on \( \Omega_1 \cap \Omega_2 \). It will hold that

\[ Lu_1 = f, \quad \text{in } \Omega_1 \]
\[ w_1 = w_2, \quad \text{on } \Gamma_1 \]
\[ w_1 = 0, \quad \text{on } \partial \Omega \cap \partial \Omega_1 \]
\[ Lu_2 = f, \quad \text{in } \Omega_2 \]
\[ w_2 = w_1, \quad \text{on } \Gamma_2 \]
\[ w_2 = 0, \quad \text{on } \partial \Omega \cap \partial \Omega_2. \]  \tag{2.4}
Conversely, it can be proved that if the above coupled system is well posed, then by solving it, the original solution of (2.1) can be recovered with \( u(x) = w_i(x) \) on \( \Omega_i \) for \( i = 1, 2 \), [5].

The Schwarz alternating method is an iterative method which is used to solve (2.1). It starts from a suitable initial guess \( u^{(0)} \) and then constructs a sequence of improved approximations \( u^{(1)}, u^{(2)}, \ldots \) by solving the block of equations (2.4) in the following way. Starting with the \( k \)th iterate \( u^{(k)} \), solve the subproblems defined on \( \Omega_1 \) and \( \Omega_2 \) successively with the most current values as boundary conditions on the interface boundaries, that means successively solving the following subproblems

\[
\begin{align*}
Lw_1^{(k+1)} &= f, \text{ in } \Omega_1 \\
w_1^{(k+1)} &= u^{(k)}|_{\Gamma_1}, \text{ on } \Gamma_1 \\
w_1^{(k+1)} &= 0, \text{ on } \partial \Omega \cap \Omega_1 \\
Lw_2^{(k+1)} &= f, \text{ in } \Omega_2 \\
w_2^{(k+1)} &= u^{(k)}|_{\Gamma_2}, \text{ on } \Gamma_2 \\
w_2^{(k+1)} &= 0, \text{ on } \partial \Omega \cap \Omega_2.
\end{align*}
\]

(2.5)

Then the iterate \( u^{(k+1)} \) is defined by

\[
u^{(k+1)} = \begin{cases} w_2^{(k+1)} & \text{on } \Omega_2 \\
\bar{w}_1^{(k+1)} & \text{on } \Omega \setminus \Omega_2.
\end{cases}
\]

This method is known as the alternating Schwarz method and it can be shown that obtained iterates \( \{u^{(k)}\} \) converge with rate \( \rho \in (0,1) \) in the norm induced by the operator \( L \) to the true solution \( u \) on \( \Omega \), i.e.

\[\|u - u^{(k)}\| \leq \rho^k\|u - u^{(0)}\|,\]

where \( \rho < 1 \) depends on the choice of \( \Omega_1 \) and \( \Omega_2 \). Below, we will prove this result using a variational approach.

To do so, let us describe the variational interpretation of the alternating Schwarz method, in which the stated convergence is shown. Later, that can immediately be extended to the finite element discretization of (2.1) given by (2.3). For each \( \Omega_i \), we define a subspace \( V_i \subset H_0^1(\Omega) \) as

\[V_i = \{v \in H_0^1(\Omega) : v = 0 \text{ in } \Omega \setminus \Omega_i\}.
\]

Now, the alternating Schwarz method can be reformulated as follows. For each subproblem \( i = 1, 2 \), find \( w_i^{(k)} \in H_0^1(\Omega_i) \) and update the current iterate \( u^{(k+\frac{1}{2})} \) as

\[
a(w_i^{(k)}, v_1 |_{\Omega_i} = (f, v_1)_{\Omega_i} - a(u^{(k)}, v_1 |_{\Omega_i}), \forall v_1 \in H_0^1(\Omega_i),
\]

\[
u^{(k+\frac{1}{2})} = u^{(k)} + \bar{w}_1^{(k)}
\]

(2.6)

\[
a(w_2^{(k)}, v_2 |_{\Omega_2} = (f, v_2)_{\Omega_2} - a(u^{(k+\frac{1}{2})}, v_2 |_{\Omega_2}), \forall v_2 \in H_0^1(\Omega_2),
\]

\[
u^{(k+1)} = u^{(k+\frac{1}{2})} + \bar{w}_2^{(k)}
\]

(2.7)

where \( \bar{w}_i^{(k)} \in V_i \) extends the local solution \( w_i^{(k)} \) outside \( \Omega_i \). Equations (2.6)-(2.7) represent the variational formulation of the alternating Schwarz algorithm, equivalent to the original one (2.5), for more details see [6]. Let \( P_i \) be the orthogonal projection operator of the space \( H_0^1(\Omega) \) onto the subspace \( V_i \). Then for any \( w \in H_0^1(\Omega) \) it holds that \( P_i w \in V_i \) satisfies

\[a(P_i w, v) = a(w, v), \forall v \in V_i,
\]

and the updates \( u^{(k+\frac{1}{2})} \) can be expressed in terms of these projection operators onto the subspaces \( V_i \). From (2.6)-(2.7) we have that the following hold

\[a(u^{(k+\frac{1}{2})} - u^{(k)}, v) = a(u - u^{(k)}, v), \forall v \in V_1, \text{ and}
\]

\[a(u^{(k+1)} - u^{(k+\frac{1}{2})}, v) = a(u - u^{(k+\frac{1}{2})}, v), \forall v \in V_2,
\]

where \( u \) is the exact solution of (2.1). Therefore, sequences \( u^{(k+\frac{1}{2})} \) and \( u^{(k+1)} \) satisfy

\[
u^{(k+\frac{1}{2})} = u^{(k)} + P_1(u - u^{(k)}), \text{ and}
\]

\[
u^{(k+1)} = u^{(k+\frac{1}{2})} + P_2(u - u^{(k+\frac{1}{2})}).
\]

(2.8)
Substituting \( u = L^{-1}f \), from equations (2.8) we get the following
\[
\begin{align*}
u^{(k+\frac{1}{2})} &= u^{(k)} + P_1L^{-1}(f - Lu^{(k)}), \\
u^{(k+1)} &= u^{(k+\frac{1}{2})} + P_2L^{-1}(f - Lu^{(k+\frac{1}{2})}).
\end{align*}
\]
(2.9)

Subtracting iterates from the true solution \( u \) and applying the equations (2.8) we get the following equation for the error \( e^{(k)} \equiv u - u^{(k)} \)
\[
e^{(k+1)} = (I - P_2)(I - P_1)e^{(k)}.
\]
Considering how this iteration operator looks like, the alternating Schwarz method is often called multiplicative Schwarz method. Following [6], here we prove that the map \((I - P_2)(I - P_1)\) is a contraction with respect to the norm generated by the operator \( L \), i.e. with respect to the norm \( \| \cdot \|_L^2 \equiv a(\cdot, \cdot) \).

**Theorem 2.1.** If \( V_1 \oplus V_2 = H^2_0(\Omega) \) then the iteration operator \((I - P_2)(I - P_1)\) is a contraction in \( H^1_0(\Omega) \) with respect to the norm generated by the operator \( L \), i.e. there exist a constant \( C_0 \geq 1 \) such that
\[
\|(I - P_2)(I - P_1)v\|_L^2 \leq \left( 1 - \frac{1}{C_0^2} \right) \|v\|_L^2, \forall v \in H^1_0(\Omega).
\]

**Proof.** Here, whenever we use the norm, we assume it is the one induced by the operator \( L \). Also, we will use the notation that \( V = H^1_0(\Omega) \). First, let us prove that there exist a constant \( C_0 \geq 1 \) such that
\[
\|v\| \leq C_0(\|P_1v\|^2 + \|P_2v\|^2)^{1/2}, \forall v \in H^1_0(\Omega).
\]
(2.10)

We assumed that \( V_1 \oplus V_2 = V \) holds. Consequently, applying the open mapping theorem to the map \( V_1 \times V_2 \to V \), defined by \( (v_1, v_2) \mapsto v_1 + v_2 \), gives the existence of \( C_0 \geq 1 \) such that for each \( v \in V \) it is possible to choose \( v_1 \in V_1 \) and \( v_2 \in V_2 \) such that \( v = v_1 + v_2 \) and
\[
(\|v_1\|^2 + \|v_2\|^2)^{1/2} \leq C_0\|v\|.
\]
(2.11)

Then for every \( v \in V \), we have the following
\[
\|v\|^2 = a(v_1, v) + a(v_2, v) = a(v_1, P_1v) + a(v_2, P_2v)
\leq (\|v_1\|^2 + \|v_2\|^2)^{1/2}(\|P_1v\|^2 + \|P_2v\|^2)^{1/2}
\leq C_0\|v\|(\|P_1v\|^2 + \|P_2v\|^2)^{1/2},
\]
where the first equality is due to \( v = v_1 + v_2 \) and the second due to the definition of the projection operators. In the first inequality we used Cauchy-Schwarz and in the second (2.11). Finally, dividing this last inequality by \( \|v\| \), we will get (2.10).

If we now apply inequality (2.10) to the vector \((I - P_1)v\), we get
\[
\|(I - P_1)v\| \leq C_0\|P_2(I - P_1)v\|,
\]
(2.12)

since for the projection operator \( P_1(I - P_1) = 0 \) holds. If \( \{x_1, \ldots, x_n\} \) is the set of orthogonal vectors in \( H^1_0(\Omega) \) than we have that \( \|\sum_{i=1}^{n} x_i\|^2 = \sum_{i=1}^{n} \|x_i\|^2 \). Therefore, since \( P_2 \) is an orthogonal projection, we have
\[
\|(I - P_1)v\|^2 = \|(I - P_2)(I - P_1)v\|^2 + \|P_2(I - P_1)v\|^2
\geq \|(I - P_2)(I - P_1)v\|^2 + \frac{1}{C_0^2}\|(I - P_1)v\|^2,
\]
where we used (2.12). Reordering and using that \( P_1 \) is an orthogonal projection, finally gives
\[
\|(I - P_2)(I - P_1)v\|^2 \leq \left( 1 - \frac{1}{C_0^2} \right) \|(I - P_1)v\|^2 \leq \left( 1 - \frac{1}{C_0^2} \right) \|v\|^2.
\]
\[\blacksquare\]
This result immediately implies that the alternating Schwarz method converges with the rate \(\rho = 1 - C_0^{-2}\). For the more detailed convergence rate estimates see [5] and [7]. There, one can find similar convergence results for a decomposition into \(M \geq 2\) subdomains and also for the finite dimensional case. It can be shown that after some coarse grid corrections, convergence rate depends only on the operator \(L\) and the size of the overlap.

The variational formulation of the alternating Schwarz algorithm (2.6) and (2.7), can be immediately adapted to the discrete finite element case just by introducing the space of finite element functions \(V_h\), and taking \(V_{i,h} \equiv V_i \cap V_h\). Since the finite element approximation of the problem (2.1) gives the algebraic system \(Au = f\) as in (2.3), we now give the alternating Schwarz algorithm in algebraic terms.

Let \(I_1\) and \(I_2\) denote the indices of the nodes in the interior of \(\Omega_1\) and \(\Omega_2\), respectively. For the overlapping subregions \(\Omega_1\) and \(\Omega_2\) we will have that \(I_1 \cup I_2 = I\) and \(I_1 \cap I_2 \neq \emptyset\), where \(I\) is the set of all indices from 1 to \(n\), and \(n\) is the total number of the internal nodes in \(\Omega\). Clearly, due to the overlap \(n_1 + n_2 > n\) also holds, for \(n_1\) is the number of the internal nodes in \(\Omega_1\). The indices are ordered such that first the nodes internal to \(\Omega_1\) but not internal to \(\Omega_2\) appear, then those corresponding to the nodes in the interior of \(\Omega_1 \cap \Omega_2\), and at the end the remaining ones.

To derive a matrix form of the alternating Schwarz algorithm (2.3), we have to define extension and restriction matrices in the following way. The matrix \(R_i\) is a \(n_1 \times n\) rectangular matrix whose action extends the vector of nodal values in the interior of \(\Omega_i\) by zeros, such that a full vector \(n \times 1\) is obtained. Therefore, given a subvector \(v_i \in H^1(\Omega_i) \cap V_h\) of length \(n_1\), we obtain the following vector in \(V_{i,h}\)

\[
(R_i v_i)_k = \begin{cases} 
(v_i)_k & \text{for } k \in I_i \\
0 & \text{for } k \in I \setminus I_i.
\end{cases}
\]

From this definition of the extension matrix, we have that the first \(n_1\) rows and columns of the matrix \(R_1 \in \mathbb{R}^{n_1 \times n_1}\) form the identity matrix. The same holds for the last \(n_2\) rows and columns of \(R_2 \in \mathbb{R}^{n \times n_2}\).

On the other hand, the transpose \(R_i^T\) of \(R_i\) is a \(n \times n_1\) rectangular matrix whose action restricts a full vector to a vector of length \(n_i\) by preserving the entries corresponding to the indices \(I_i\). When formulating the alternating Schwarz, the assumption is that each \(V_{i,h}\) is a subspace in \(\mathbb{R}^n\) of dimension \(n_i\), and that the columns of the restriction matrix \(R_i\) form a basis for \(V_{i,h}\), so that \(\text{Range}(R_i) = V_{i,h}\).

Therefore, we have assumed that \(V_{1,h} \oplus V_{2,h} = \mathbb{R}^n\), which will ensure the convergence given in Theorem 2.1.

Matrix \(A\) in the system (2.3), often called global stiffness matrix, contains two principal submatrices \(A_1\) and \(A_2\) formed by the first \(n_1\) rows and columns, and the last \(n_2\) rows and columns of \(A\), respectively. These submatrices are local stiffness matrices for the subdomains \(\Omega_1\) and \(\Omega_2\). They are related to \(A\) by the following algebraic equations

\[
A_1 = R_1^T A R_1 \quad \text{and} \quad A_2 = R_2^T A R_2.
\]

From the variational formulation of the alternating Schwarz algorithm (2.6) and (2.7), we obtain the discrete version of the alternating Schwarz algorithm, by replacing the operators with the corresponding matrices, [6]. To solve \(Au = f\), starting from any suitable initial guess \(u^{(0)}\), the discrete alternating Schwarz algorithm generates a sequence \(u^{(1)}, u^{(2)}, \ldots\) by the following equations

\[
\begin{align*}
    u^{(k+\frac{1}{2})} &= u^{(k)} + R_1 A_1^{-1} R_1^T (f - A u^{(k)}), \\
    u^{(k+1)} &= u^{(k+\frac{1}{2})} + R_2 A_2^{-1} R_2^T (f - A u^{(k+\frac{1}{2})}).
\end{align*}
\]

This corresponds to a generalisation of the block Gauss-Seidel iteration for solving (2.3). If we now replace \(f = Au\) and introduce the discrete projection operators onto the space \(V_{i,h}\) for \(i = 1, 2\) as

\[
P_i \equiv R_i A_1^{-1} R_i^T A,
\]

equations (2.13) can be rewritten as

\[
\begin{align*}
    u^{(k+\frac{1}{2})} &= u^{(k)} + P_1 (u - u^{(k)}), \\
    u^{(k+1)} &= u^{(k+\frac{1}{2})} + P_2 (u - u^{(k+\frac{1}{2})}).
\end{align*}
\]

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A simple substitution gives that the error equation is
\[ e^{(k+1)} = (I - P_g)(I - P_I)e^{(k)}, \] (2.14)
and therefore the convergence is governed by the iteration matrix \((I - P_g)(I - P_I)\).

3 Domain decomposition and particle-to-continuum coupling

In section 2 we discussed the results in the classical continuum-to-continuum domain decomposition framework given in Schwarz formulation for overlapping subdomains. Now, we will use the alternating Schwarz algorithm in a particle-to-continuum context. We will use it to couple a particle with a continuum model, where the latter is supposed to be discretized by finite elements. To do this, particles, e.g. atoms, will be treated as finite element nodes in the overlap region when needed, and vice-versa. In particular, the matrix formulation of the alternating Schwarz method given by (2.13) will be considered.

Before solving the coupling problem, let us first describe the global particle and the global continuum model which we want to couple. Global in the sense that a model is considered on the whole domain \(\Omega\). The global particle domain which we will consider, consists of a one, two or three dimensional Bravis-like lattice of atoms, \([4]\). We assume that all atoms interact with their nearest and second-nearest neighbours only. The interaction between the atoms takes place along a spring, so that a system, in physics known as an atom-spring network, is defined. If we have \(n\) atoms in a global atomistic model, it is described by the following linear system
\[ K^a u^a_g = f^a, \] (3.1)
where \(K^a \in \mathbb{R}^{n \times n}\) is the stiffness matrix of the atom-spring network, and the vector \(u^a_g \in \mathbb{R}^n\) contains unknown atomistic positions after the force \(f^a_g \in \mathbb{R}^n\) is applied. Our main goal is to find unknown \(u^a_g\), but not by solving this global atomistic model (3.1).

Let us give here an example how the linear system is obtained from one-dimensional atom-spring model with \(r = 2\). If \(r = 2\) all atoms are connected to their nearest and second-nearest neighbours only. Assume that the nearest-neighbour atoms are bounded by a spring of stiffness \(k_1\), and the second-nearest by a spring of stiffness \(k_2\). Also, the leftmost and the rightmost atoms are held fixed corresponding to the Dirichlet boundary conditions. Let \(h\) be the distance between two atoms and \(u_l = lh\), \(l \in \mathbb{Z}\) the atomistic positions. Then the interaction between atoms is described by the following potential function which is a function of the distance \(h\)
\[ \Pi = \sum l \left[ \frac{k_2}{2} (u_l - u_{l-2})^2 + \frac{k_1}{2} (u_l - u_{l-1})^2 + \frac{k_1}{2} (u_{l+1} - u_l)^2 + \frac{k_2}{2} (u_{l+2} - u_l)^2 \right]. \] (3.2)
To obtain the stiffness matrix \(K^a\) corresponding to the global atomistic model given by (3.1), the potential (3.2) is differentiated with respect to the atomic positions. Hence, we have that
\[ (K^a)^{i,j} = \frac{\partial^2 \Pi}{\partial u_i \partial u_j}, \]
for \(i, j = 1, \ldots, n\).

On the other hand, we have a corresponding global one, two or three-dimensional continuum model. Indeed, it can be shown that up-scaling the considered global atomistic model via an appropriate limiting process recovers an associated continuum partial differential equation, \([4]\). Then, the recovered PDE is discretized by the finite element method and a global finite element model is obtained. Note here that we have gone from a nonlocal atomistic model to a local finite element one. Namely, in real materials interatomistic potentials span over many atoms and in finite element discretization basis functions usually have local support. After appropriate up-scaling and discretizing, we will again have a sparse linear system for the global continuum model, as the one given in (2.3). Let us write here the corresponding linear system for the global finite element model as
\[ K^{fe} g \cdot u^{fe}_g = f^{fe}_g, \] (3.3)
where \(K^{fe}_g \in \mathbb{R}^{n \times n}\), \(u^{fe}_g \in \mathbb{R}^n\) and \(f^{fe}_g \in \mathbb{R}^n\), since we assume that there is the same number of finite element nodes in the global finite element model as atoms in the global atomistic model, \(n\).
In the one-dimensional case, it can be shown that the corresponding differential equation obtained by letting $h \to 0$ in the atomistic model with the potential energy given by (3.2) reads

$$\frac{d}{dx} \left( k_c \frac{du}{dx} \right) = f,$$

for a density function $u$ and $k_c = k_1 + 4k_2$. For more details on one-dimensional models see [8].

So far, we have defined the global atomistic and continuum models on the whole domain $\Omega$. However, in our coupled model neither of these models will be solved on the whole domain $\Omega$. Indeed, let us assume that the whole domain is divided in five disjoint subregions $\Omega = \bigcup_{i=1}^{5} \Omega_i$, where each $\Omega_i$ has cardinality $n_i$ so that $n = \sum_{i=1}^{5} n_i$. Let $\Omega^a = \Omega \setminus \Omega_5$ and $\Omega^{fe} = \Omega \setminus \Omega_1$ be subdomains such that $\{\Omega^a, \Omega^{fe}\}$ form an overlapping decomposition of $\Omega$ with an overlap $\cup_{i=2}^{4} \Omega_i$ and corresponding interior “boundaries” $\Gamma^a = \Omega_4$ and $\Gamma^{fe} = \Omega_2$. This subdomain construction in the one-dimensional case is sketched in the Figure 2.

![Figure 2: The overlapping decomposition of domain $\Omega$ in one-dimensional case consists of $\{\Omega^a, \Omega^{fe}\}$. Here, circles represent atoms and squares finite element nodes. This graphic is taken from [4].](image)

In our coupled model, an atomistic model is defined on $\Omega^a$ and a finite element model on $\Omega^{fe}$. Therefore, we will couple the following two systems

\begin{align*}
K^a u^a &= f^a, \quad (3.4) \\
K^{fe} u^{fe} &= f^{fe}, \quad (3.5)
\end{align*}

which are obtained by restricting the systems (3.1) and (3.3) to the subdomains $\Omega^a$ and $\Omega^{fe}$, respectively.

When using the alternating Schwarz to solve our coupled model, first we solve (3.4) in the atomistic subdomain $\Omega^a$, so that the atoms in $\Gamma^a$ are held fixed according to the positions of finite element nodes, i.e. subject to a Dirichlet boundary condition. Then we solve (3.5) in $\Omega^{fe}$ by holding the atoms in $\Gamma^{fe}$ fixed according to the positions of corresponding atoms. This alternation will be performed until convergence, and we will use a sufficiently small change in the global solution vector as a stopping criterion. Here, the size of $\Omega_3$ can be altered to control the size of the subdomain overlap and therefore change the rate of convergence. It is important that the subdomain $\Omega_4$, corresponding to the interior boundary $\Gamma^a$, must be of width at least equal to the cutoff radius $r$ used in the atomistic model. This is to prevent atoms close to $\Gamma^a$ from acting as they are in the presence of a surface, since this boundary $\Gamma^a$ is just artificial.

Now, we will use the matrix form of alternating Schwarz to solve (3.4) and (3.5) as a coupled system. We introduce extension operators $R_1$ and $R_2$ and obtain $K^a$ and $K^{fe}$ from the global stiffness matrices $K^g_a$ and $K^g_{fe}$, respectively. Following what has been done in section 2, we write extension matrices $R_1 \in \mathbb{R}^{n \times (n_1+n_2+n_3)}$ and $R_2 \in \mathbb{R}^{n \times (n_3+n_4+n_5)}$ as

\begin{align*}
R_1 &= \begin{bmatrix} I & 0 & 0 \\
0 & I & 0 \\
0 & 0 & I \\
0 & 0 & 0 \\
0 & 0 & 0 \end{bmatrix}, & R_2 &= \begin{bmatrix} 0 & 0 & 0 \\
0 & 0 & 0 \\
I & 0 & 0 \\
0 & I & 0 \\
0 & 0 & I \end{bmatrix},
\end{align*}

where $I$ and 0 are identity and zero matrices of appropriate dimensions. Now we can obtain stiffness matrices corresponding to subdomains $\Omega^a$ and $\Omega^{fe}$ by the following equations

\begin{align*}
K^a &= R_1^T K^g_a R_1, \\
K^{fe} &= R_2^T K^g_{fe} R_2.
\end{align*}
Then, similar to (2.13), the $k^{th}$ iteration of the alternating Schwarz algorithm reads

$$u^{(k+\frac{1}{2})} = u^{(k)} + R_1(K^{-1})_{12} f^{(a)}_g - K^{-1}_g u^{(k)},$$

$$u^{(k+1)} = u^{(k+\frac{1}{2})} + R_2(K^{fe})^{-1} R^T_2 (f^{fe}_g - K^{fe}_g u^{(k+\frac{1}{2})}).$$

By introducing projection matrices $P^a = R_1(K^{-1})_{12} K^{-1}_g$ and $P^{fe} = R_2(K^{fe})^{-1} R^T_2 K^{fe}_g$, analogously to (2.14), we will have the following equations

$$u^{(k+\frac{1}{2})} = u^{(k)} + P^a (u^{(k)}_g - u^{(k)}),$$

$$u^{(k+1)} = u^{(k+\frac{1}{2})} + P^{fe} (u^{(k)}_g - u^{(k+\frac{1}{2})}).$$

Defining the error at the $k^{th}$ step as $e^{(k)} \equiv u^{(k)} - u^{(k)}_g$ and the vector $d$ as the difference of the global finite element and the global atomic solution, i.e., $d \equiv u^{fe}_g - u^{a}_g$, we get that the error satisfies the following equation

$$e^{(k+1)} = (I - P^{fe})(I - P^a)e^{(k)} + P^{fe}d.$$ (3.8)

Note that this error equation differs from the error equation (2.14) which we had in the classical alternating Schwarz, by the extra term $P^{fe}d$. Hence, the spectral radius of the matrix $(I - P^{fe})(I - P^a)$ being less than 1 is not enough for the convergence of the alternating Schwarz method in the context of particle-to-continuum coupling. Still, we can provide the following error analysis.

First of all, note that Theorem (2.1) does not directly apply here, because now the projection matrices $P^a$ and $P^{fe}$ are obtained from different global matrices and bilinear forms induced by $K^{a}_g$ and $K^{fe}_g$ would differ. Rather, the following error estimate was proved in [4].

**Theorem 3.1.** Assume that the iteration matrix $(I - P^{fe})(I - P^a)$ has the eigendecomposition $V\Lambda V^{-1}$ such that $\sigma \neq 1$ is the spectral radius of $\Lambda$ and $\kappa$ is the condition number of the eigenvector matrix $V$. Then the 2-norm of the error (3.8) can be bounded as follows

$$\|e^{(k+1)}\| \leq \sigma^{k+1} \kappa \left( \|e^{(0)}\| - \frac{\|P^{fe}d\|}{1 - \sigma} \right) + \kappa \frac{\|P^{fe}d\|}{1 - \sigma}.$$ (3.9)

**Proof.** Given the eigendecomposition of the iteration matrix and the error equation equation (3.8), a simple substitution yields

$$e^{(k+1)} = V\Lambda^{k+1}V^{-1}e^{(0)} + \sum_{i=0}^{k} V\Lambda^{i}V^{-1}P^{fe}d.$$ 

Since we use the 2-norm, we have $\|\Lambda\|^{k+1} = \sigma^{k+1}$. Also $\kappa = \|V\|\|V^{-1}\|$ holds, and therefore, by taking norms we get

$$\|e^{(k+1)}\| \leq \kappa\sigma^{k+1}\|e^{(0)}\| + \kappa\|P^{fe}d\| \sum_{i=0}^{k} \sigma^i$$

$$= \kappa\sigma^{k+1}\|e^{(0)}\| + \kappa\|P^{fe}d\| \frac{1 - \sigma^{k+1}}{1 - \sigma},$$

which finishes the proof. 

Considering the bound (3.9), we have that if for the spectral radius of $\Lambda$ the condition $\sigma < 1$ holds, then the first term in (3.9) goes to zero as $k \to \infty$. The second term in (3.9) is independent of $k$ and it remains. Hence, the error stays limited by the measure of the difference between the global atomistic and the global finite element model, which becomes smaller as the continuum model is the better approximation for the atomistic model.

Following the results given in [9], it is possible to prove that $\sigma$ is equal to the spectral radius of submatrix $P_{x,y}^{fe}$, where a subscript $x$ in the matrix $P_x$ gives the corresponding position of this submatrix in the projection matrix $P$. For more details see [4]. Still, this does not prove that $\sigma < 1$. In
the one-dimensional case, numerical results support that $\sigma < 1$ holds. Moreover, it decreases as the size of the overlap increases, which improves the rate of convergence. This is captured in Table 1.

In Table 1, the results of testing the alternating Schwarz method on the one-dimensional coupled atomistic-to-continuum model are shown. We have tested the model which was motivated by descriptions of models used in [4] and [8]. The corresponding global atom-spring model with $r = 2$, which we used, consists of $n = 105$ atoms, where the two leftmost and two rightmost atoms are held fixed corresponding to the Dirichlet boundary conditions. Also, in the corresponding global finite element model, there are 105 nodes with othermost nodes fixed.

In the finite element model, the piecewise linear basis functions are used. Further, in our coupled model, the constant point force on the atom in the pure atomistic subdomain is applied and the size of the overlap is changed by the parameter $\delta$. Here, $\delta$ is the number of overlapping atoms/nodes to the left and to the right of the centred atom/node, so that $n_3 = 2\delta + 1$.

In all tested cases, $\Gamma^a$ and $\Gamma^{fe}$ have 2 atoms and 2 nodes, respectively, i.e. $n_2 = n_4 = 2$. As noted before, the stopping criterion which we use is a sufficiently small change in the global solution vector $u$. Particularly, stopping criterion is $\|u^{(k)} - u^{(k-1)}\| < \varepsilon$ with $\varepsilon = 10^{-8}$.

Regarding the analysis of the second term in the bound (3.9), in [4] the value of $\|P^{fe}d\|$ is considered. If we brake vector $d$ into five pieces according to our decomposition of the global domain $\Omega_1, \ldots, \Omega_5$, we can see that in $\|P^{fe}d\|$ the part $d_1$ does not appear since the matrix $P^{fe}$ operates only on $\Omega^{fe}$-part. The vector $d_1$ represents the difference of the global atomistic and finite element solutions in the purely atomistic subdomain $\Omega_1$. We expect it to be different than 0 as we have chosen $\Omega_1$ to be purely atomistic in the coupled model because a finite element solution in this domain does not produce acceptable results. However, $d_1$ has no influence on $\|P^{fe}d\|$, so we do not mind if $d_1 \neq 0$. For the remaining parts of $d$: $\{d_i, i = 2, \ldots, 5 \}$, numerical results in the one dimensional case, show that they are small enough to influence $\|P^{fe}d\|$ to be considerably smaller then the error. Moreover, in this special case, numerical results suggest that the second term in (3.8) and (3.9) disappears. This is also captured in Table 1.

<table>
<thead>
<tr>
<th>$\delta$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$|u - u^a|$</td>
<td>$1.5161 \times 10^{-10}$</td>
<td>$9.7438 \times 10^{-10}$</td>
<td>$7.3157 \times 10^{-10}$</td>
<td>$6.3856 \times 10^{-10}$</td>
<td>$5.9744 \times 10^{-10}$</td>
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<tr>
<td>$N_{it}$</td>
<td>55</td>
<td>33</td>
<td>25</td>
<td>20</td>
<td>17</td>
</tr>
<tr>
<td>$|P^{fe}d|$</td>
<td>$3.6302 \times 10^{-08}$</td>
<td>$3.6650 \times 10^{-08}$</td>
<td>$3.6994 \times 10^{-08}$</td>
<td>$3.7335 \times 10^{-08}$</td>
<td>$3.7673 \times 10^{-08}$</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>0.9177</td>
<td>0.8480</td>
<td>0.7840</td>
<td>0.7247</td>
<td>0.6697</td>
</tr>
<tr>
<td>$t$</td>
<td>0.2061</td>
<td>0.1297</td>
<td>0.0611</td>
<td>0.0551</td>
<td>0.0358</td>
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</table>

Table 1: The one-dimensional atomistic-to-continuum model solved by the alternating Schwarz method. Here, $N_{it}$ is the number of iterations and $t$ is the computational time in seconds, which is calculated as the average out of 10 testings.

### 3.1 Non-matching finite element grid and particle lattice

Here, we will consider the case when non-matching grids are used in the one-dimensional coupled model. After all, the reason of solving the coupled model instead of the pure atomistic model is to reduce the computational cost of the atomistic simulations. In order to achieve this, the finite element grid can be made coarser than the atomistic lattice. Hence, the smaller number of finite element nodes will be involved and the coupled model will be more efficient, but probably less accurate. Bellow, this will be captured trough the numerical results in our one-dimensional coupling model. We consider the case where the atoms and the finite element nodes are still on top of each other in the overlap, but now the distance between two neighbouring nodes is double the distance between two neighbouring atoms. This is shown in the Figure 3.

![Figure 3: The overlapping decomposition of domain $\Omega$ in the one-dimensional coupling model with non-matching finite element grid and atomistic lattice.](image-url)
Introducing the coarser finite element grid requires additional grid-transfer operators. In the equation of the alternating Schwarz algorithm (3.7), which refers to the finite element part, first one needs the transfer operator $T_1$ to go from the finer atomistic lattice to the coarser finite element grid. Further, the transfer operator $T_2$ is needed to interpolate the values from the positions of atoms onto the positions of finite element nodes, i.e., to go from the coarser finite element grid to the finer atomistic lattice. The grid-transfer operator $T_1$ can be written as a transpose of the interpolation operator onto.

The transfer operator $T_2$ where the matrix $\hat{R}$, corresponding to the subdomain $\Omega$, is obtained from the global finite element matrix $K_{fe} \in \mathbb{R}^{n \times n}$ by the following equation

$$
\hat{R} = (T_2 R_2) K_{fe} T_2 R_2.
$$

This matrix $\hat{R} \in \mathbb{R}^{(n_3+n_4+n_5)/2 \times (n_3+n_4+n_5)/2}$ corresponds to the finite element model where the distance between two neighbouring nodes is double the distance we had in matching grid case. The projection matrix corresponding to the finite element subdomain is

$$
\hat{P} = T_2 R_2 (K_{fe})^{-1} \left( \frac{1}{2} R_2 T_2 \right)^T K_{fe}.
$$

Hence, instead of the equation (3.8) which we had in the matching grid case, now we obtain

$$
e^{(k+1)} = (I - \hat{P}) (I - P) e^{(k)} + \hat{P} d.
$$

However, in this case, numerical results do not support that spectral radius $\hat{\sigma}$ of $(I - \hat{P}) (I - P)$ is strictly less than 1. Moreover, from the numerical testing, we get that $\hat{\sigma} = 1$, which does not allow us to use analysis we had in the case with matching grids. The numerical results of testing our one-dimensional coupling model described previously, with the change of the non-matching grids, are given in Table 2.

<table>
<thead>
<tr>
<th>$\delta$</th>
<th>0</th>
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<th>3</th>
<th>4</th>
</tr>
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<td>51</td>
<td>41</td>
<td>35</td>
</tr>
<tr>
<td>$\hat{\sigma}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$t$</td>
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<td>0.2065</td>
<td>0.1757</td>
<td>0.1484</td>
<td>0.0894</td>
</tr>
</tbody>
</table>

Table 2: The non-matching grid case. Again, $N_i$ is the number of iterations and $t$ denotes the computational time in seconds, as the average out of 10 testings.

From the numerical experiments, it can be concluded that using coarser finite element grid, and hence smaller number of finite element nodes, gives less accuracy but faster execution of the alternating Schwartz method in the atomistic-to-continuum context. Although we got that $\hat{\sigma} = 1$, these numerical results suggest the convergence of the method. In Figure 4, the difference $\| u^{(k+1)} - u^{(k)} \|$ throughout iterations is shown. This again suggests the convergence.
Figure 4: The difference \( \| \mathbf{u}^{(k+1)} - \mathbf{u}^{(k)} \| \) throughout iterations of the alternating Schwartz method tested on the one-dimensional coupled model with non-matching finite element grid and atomistic lattice.

References


