

Recent advances and challenges in interfacial MD-FE coupling for amorphous polymers

M. Ries^{1,*}, Y. Jain², F. Müller-Plathe², S. Pfaller¹

¹ Institute of Applied Mechanics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

² Department of Chemistry, Technische Universität Darmstadt, Germany

* maximilian.ries@fau.de

Keywords: atomistic-continuum coupling, amorphous polymer, concurrent multiscale simulation.

Summary: *Polymers are a highly versatile class of materials that can exhibit remarkable properties, especially in combination with nano-sized filler particles. However, the extremely small length scales pose major problems for the experimental investigation of the complex matrix-filler interactions. Instead, numerical methods can be used, of which multiscale approaches are particularly noteworthy since they, i.a., exploit the accuracy of particle-based methods while maintaining the efficiency of continuum mechanics. The complexity of these approaches lies in the design of the scale coupling that has to avoid coupling artifacts that might distort the results while being computationally efficient. In this contribution, we introduce an MD-FE coupling via an interface for amorphous polymers. The approach relies on padding atoms as particle representations of the continuum enabling interactions with the actual particles. We evaluate the new coupling scheme with a toy system of amorphous polystyrene and carefully discuss the system's behavior during an MD-FE equilibration run. We observe considerable oscillations of our sample system, which we attribute to a combination of the rigid coupling condition and insufficient force correction. Our results indicate that an interfacial coupling scheme cannot capture the dynamic behavior of amorphous polymers and emphasizes the need for an interphase-based coupling.*

1. INTRODUCTION

Polymers and their composites are highly versatile materials that are already used in a plethora of applications. In particular, nano-sized fillers have yielded remarkable improvements in mechanical [1, 2, 3], electrical [4], thermal [5, 6], and optical [7] properties which is why many researchers have been addressing this subject [8]. However, the extremely small length scales pose major challenges to identify the effects of the nanoparticles experimentally; hence, numerical methods are utilized instead. In many cases, conventional numerical approaches cannot be used: Particle-based methods are usually computationally too expensive, while continuum mechanics simply cannot resolve the atomistic scale. To circumvent these problems, multiscale methods have been developed combining the computational efficiency of continuum mechanics with the molecular accuracy of particle-based methods and thus facilitate the analysis of polymer nanocomposites [9].

These multiscale methods can be divided into sequential and concurrent techniques [10]. The former determines quantities on the fine scale that are applied in a subsequent analysis on the coarse scale. As an example, a material characterization based on molecular dynamics (MD) pseudo-experiments [11, 12] is used to subsequently calibrate a continuum mechanical constitutive law [13] enabling the analysis of significantly larger samples, e.g., with the finite element method (FE). In contrast, concurrent multiscale approaches apply both resolutions simultaneously and are thus suited for the analysis of complex problems. For example, the Capriccio method [14, 15, 16] couples MD and FE via a handshake region where so-called anchor points are introduced as information transmitters between the two descriptions. The method has been successfully applied to identify the property gradients forming around nano-sized filler particles embedded in an amorphous polymer matrix [17, 18, 19]. Furthermore, the Capriccio method has recently been extended [20] to study crack propagation in atactic polystyrene [21]. The Capriccio method established the scale transition via a handshake region where both descriptions overlap, which is also referred to as interphase coupling [22]. Other well-known representatives of this category are the Arlequin method [23, 24], the Bridging Domain method [25, 26], and the Atomistic-to-Continuum method [27, 28]. In case of an interface coupling, in contrast, there is no such an overlapping region, but only a boundary layer that separates the two levels of description. This concept is implemented i.a. in the Quasicontinuum method [29, 30] and the FE2AT method [31], which are mainly used for crystalline materials. However, even with interface coupling, a transition region (padding region) may be necessary if a local material representation, e.g., classical continuum mechanics, is coupled to a non-local description, where a material point interacts not only with its immediate surrounding but with all neighbors within a certain cut-off radius [22, 10].

So far, the Capriccio method requires to cut the polymer chains in order to provide non-periodic boundary conditions for the particle domain. However, it has already been shown that modifying the molecular weight has a considerable impact on the mechanical properties of amorphous thermoplastics and should thus be avoided [32]. Therefore, the question arises whether an interface coupling approach - where a padding region prevents chain cutting - can

provide for a physically more sound MD-FE coupling scheme.

In this contribution, we implement such an interface coupling based on [33] and evaluate its performance with MD-FE equilibration simulations. However, it turns out that this approach is numerically unstable and cannot cope with the dynamics of an amorphous thermoplastic at finite temperature.

2. SIMULATION METHOD

In our new coupling approach, we consider the discrete particle domain Ω^d and the continuum Ω^c as visualized in Figure 1. The bulk of the particle domain Ω^{md} is treated with classical MD solving Newton's equations of motion. In the peripheral zone Ω^{dpd} we introduce additional dissipative and random forces F^D and F^R by means of dissipative particle dynamics (DPD) [34, 35, 36]:

$$\begin{aligned} \mathbf{f} &= [F^C + F^D + F^R] \hat{\mathbf{r}}_{ij} \text{ with} & (1) \\ F^D &= -\gamma w^2(r) [\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij}], \\ F^R &= \sigma w(r) \sqrt{\alpha(\Delta t)}, \text{ and} \\ w(r) &= 1 - \hat{\mathbf{r}}_{ij} r_c^{-1}. \end{aligned}$$

Since the friction coefficient γ and the random noise amplitude σ are linked to the temperature T via the dissipation-fluctuation theorem [35]

$$\sigma^2 = 2\gamma k_B T, \quad (2)$$

the DPD region Ω^{dpd} serves as a canonical thermostat for Ω^d [37]. Furthermore, the stochastic nature of DPD minimizes the influence of the coupling interface on the polymer bulk Ω^{md} .

The continuum Ω^c is discretized by FE and contains the padding region Ω^p . All polymer beads that protrude into Ω^c are considered as padding atoms, which can be interpreted as a particle representation of the continuum allowing interaction with the particle domain. They are embedded into the continuum and follow the deformation field of the FE mesh. Hence the interactions between the padding atoms are already included in the continuum description, and thus they must only interact with the actual particles in Ω^d . The resulting forces on the padding atoms are applied as additional external loads to the continuum, affecting its displacement field. Consequently, the system has to be solved in a staggered way by alternately simulating the continuum and particle subsystems, similarly to the Capriccio method [14]. The positions of padding atoms are only updated in the FE step while they remain spatially fixed during the MD run to confine the actual particles. These MD-FE iterations are repeated until the coupled system converges to an overall equilibrium.

By applying non-periodic boundary conditions to the particle domain, we create a free surface and thus change the physics of our sample. To compensate for the surface tension effect, we mimic the continuation of the particle system with the padding atoms. However, these surface effects are not accounted for in conventional continuum mechanical constitutive laws, and

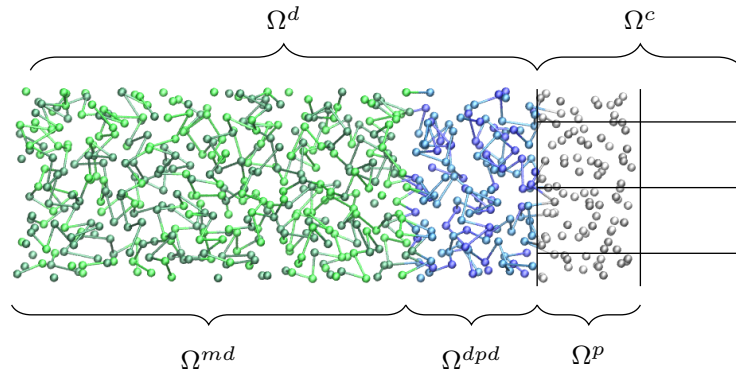


Figure 1. Schematic setup: Particle domain Ω^d treated with MD and DPD in Ω^{md} and Ω^{dpd} , respectively; continuum Ω^c discretized with FE including padding atoms located in Ω^p .

thus the forces on the padding atoms (padding forces) calculated in the MD simulation cannot be transferred directly to the continuum. Instead, we need to split them into two parts

$$\mathbf{f}^{FE}(t) = \mathbf{f}^p(t) - \mathbf{f}^{surf} \quad (3)$$

where only $\mathbf{f}^{FE}(t)$ is applied to the continuum since the static contribution \mathbf{f}^{surf} compensates for the surface tension. A numerical evaluation scheme is required since this force split cannot be calculated analytically (cf. Section 3).

The padding forces are then projected onto the FE nodes using the FE shape functions and are thus handled as external loads by a standard FE implementation. After solving the FE system, the new padding atom positions are interpolated from the obtained nodal displacements via inverted shape functions.

3. SAMPLE PREPARATION AND COMPUTATIONAL DETAILS

We use atactic polystyrene at coarse-grained (CG) resolution as a simple model system for the first evaluation of our approach. The CG scheme substitutes the styrene monomers with so-called superatoms, and the associated bond, angle, and nonbonded potentials were derived by Qian et al. [38] via Iterative Boltzmann Inversion [39]. This model is well-established and has been used to reproduce polymer dynamics [40], study polymer chain growth [41], and analyze polymer nanocomposites [42, 43, 44].

We equilibrate a large polystyrene sample under periodic boundary conditions (PBC) and carve out a cubic subsystem with an edge length of 240 Å, comprising around 90 000 atoms, which is discussed in more detail in [45]. We assign the particles in concentric cubic shells around the MD domain to the DPD and padding region, as shown in Figure 2. Consequently, the padding atoms possess the same density as the bulk polymer, which allows us to use the above-cited CG potentials for the interaction between Ω^d and Ω^p .

The thickness of the padding region corresponds to the cutoff radius of the nonbonded interactions of 15 Å, and the DPD region has a width of 20 Å [45]. In the DPD region we employ

DPD (1) to maintain a temperature of 100 K with a friction coefficient of $\gamma = 14.395 \frac{\text{kcal fs}}{\text{mol \AA}^2}$ (cf. Table 1). For the conservative forces in (1) we use the same potentials as in the inner MD region rather than the softer potentials usually related to DPD [37].

This particle setup is embedded into a hollow continuum cube with an edge length of 300 Å containing all padding atoms (cf. Figure 2). Rigid body motions are suppressed by applying Dirichlet boundary conditions to surface nodes. For the minimal constraints, only 6 degrees of freedom distributed over 3 nodes have to be fixed, while all surface nodes are clamped for maximum constraints. We employ Hooke's linear elastic constitutive law [46] for the FE domain with Young's modulus $E = 827 \text{ MPa}$ and Poisson's ratio $\nu = 0.3$ [45, 15, 43].

Since all particles are extracted from an equilibrium state, we assume the portion of the padding forces applied to the continuum to vanish: $\mathbf{f}^{FE} = \mathbf{0}$. Therefore, we can identify \mathbf{f}^{surf} as the time average of the padding forces over a long MD run with spatially fixed padding atoms. We introduce an observation region Ω^{obs} (cf. Figure 2) to directly compare quantities such as stress or density with a periodic reference solution [45].

All particle-based simulations are carried out in LAMMPS [47] while an in-house code implemented in Matlab [48] is used to solve the FE problem.

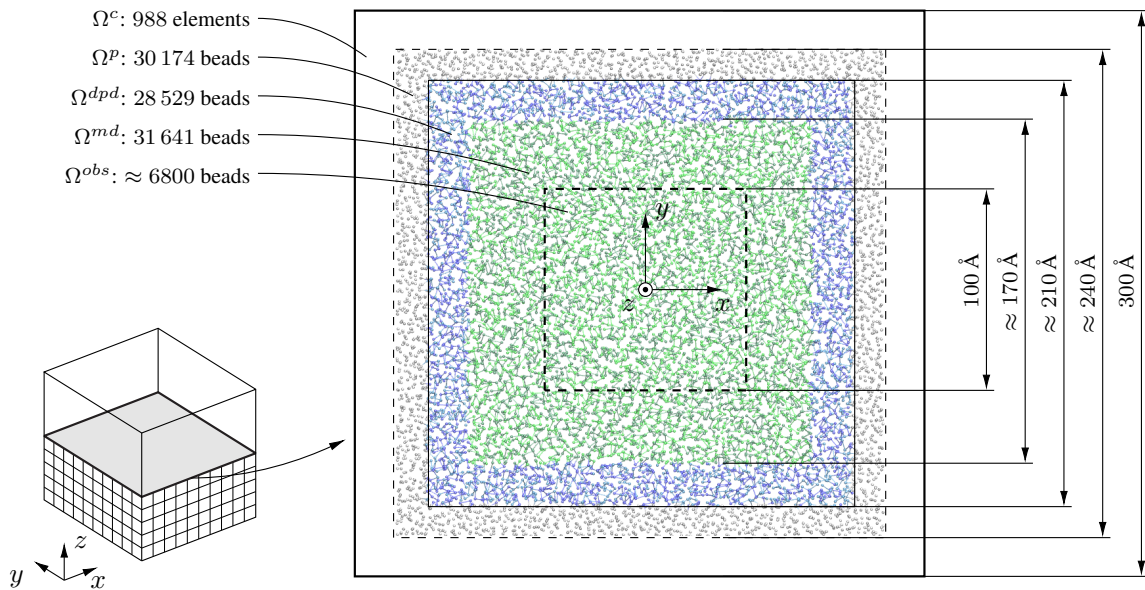


Figure 2. Coupled 3D simulation setup: the MD region Ω^{md} surrounded by the DPD region Ω^{dpd} coupled to the continuum Ω^c with the subset Ω^p containing the padding atoms; The observation region Ω^{obs} provides comparison with the PBC reference system [45]; (visualized with VMD [49]).

4. RESULTS

First, we need to identify the forces \mathbf{f}^{surf} responsible for suppressing any surface effects, and thus we equilibrate the particle region with an MD calculation over 1 000 000 timesteps with

Table 1. Simulation parameters.

DPD friction coeff. γ	14.393 kcal fs mol ⁻¹ Å ⁻²
time step Δt	5 fs
temperature T	100 K
FE Young's modulus E	827 MPa
FE Poisson's ratio ν	0.3

spatially fixed padding atoms. We average the padding forces over the last 500 000 timesteps and obtain \mathbf{f}^{surf} for each padding atom. The projection of these contributions onto the FE nodes allows us to computationally efficiently evaluate the force correction (3) at the nodal level. During this initial equilibration, the mass density of the system remains slightly below ($\approx 0.3\%$) the PBC reference solution, as shown in Figure 3 (a). Furthermore, the potential energy of the system (Figure 3 (c)), and in particular the contribution of the interactions with the padding atoms (Figure 3 (b)), remain constant, which proves that our system is still in equilibrium. Therefore, the time averaging of \mathbf{f}^{surf} in this period is justified. Figure 3 (d) demonstrates that the DPD-based thermostat can control the temperature despite the introduction of the spatially fixed padding atoms, for which $T = 0$ K.

Having obtained \mathbf{f}^{surf} we can deploy our staggered MD-FE solution scheme. The application of minimum constraints on the FE surface nodes cannot prevent rigid body motions of the whole system, which are nonphysical. This observation is in contrast to the interphase coupling of the Capriccio method, where minimal boundary conditions are sufficient [15]. Most likely, the net forces of the particle region after force correction induce a rotation, which the FE cannot counteract in this early stage of the MD-FE equilibration. For this reason, we apply maximum constraints to the system by spatially fixing all FE surface nodes. We perform 60 MD-FE iterations, each comprising $n^{iter} = 50\,000$ timesteps. The padding forces $\mathbf{f}^p(t)$ are averaged over the last $\frac{2}{3}$ of each iteration (33 000 timesteps) and corrected according to (3) with the previously identified \mathbf{f}^{surf} . However, this causes the system to oscillate around the reference density after less than 10 MD-FE iterations, which is evident from the curves of density and stress in Figure 4 (a) and (c), respectively. It appears that the padding atoms alternate between two stable states of equilibrium, leading to alternating expansion and compression of the particle region. After the initial swing-in, the padding energy in Figure 4 (b) is continuously minimized to about 12 200 kcal mol⁻¹ during the MD time step integration and increases again strongly after updating the padding atom positions in the subsequent FE step. This implies that the continuum overcompensates the adjustment of the padding atoms and thus causes persistent oscillation. Consequently, the forces acting on the continuum are too large, which could be due to an insufficient correction using the static forces determined in advance. Additionally, applying the MD potentials directly to the padding atoms might result in a too rigid coupling, especially compared to the soft harmonic coupling potentials of the Capriccio method [37]. Ultimately, the dissipation within the DPD region is not sufficient as inherent damping to dissipate and ul-

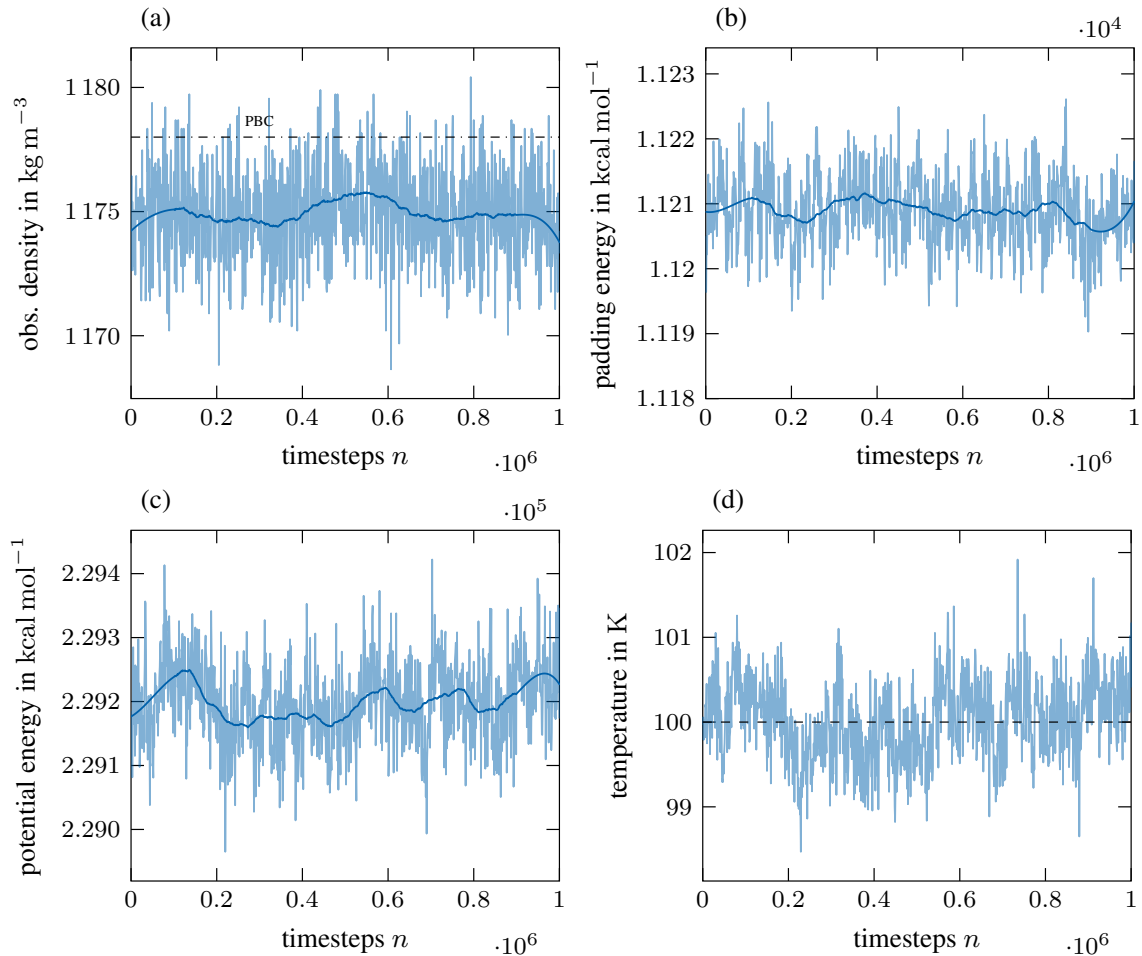


Figure 3. Initial MD equilibration: evolution of (a) density in observation region, (b) padding energy, (c) potential energy, and (d) temperature; PBC reference from [45].

timately suppress these oscillations. This is clearly illustrated in Figure 4 (d), as the thermostat can no longer maintain the temperature in the usual range of ± 2 K in these conditions. A doubling of the computed timesteps per MD-FE iteration exposes the same trends (cf. Figure 4), and confirms that the observed problem is systematic.

5. CONCLUSION

In this contribution, we present an interface-based FE-MD coupling for amorphous polymers. We introduce padding atoms for the information transfer and to enable the transition from the nonlocal particle to the local continuum description. These padding atoms follow the continuum deformation and interact with the actual particles. Since forces suppressing surface effects from the particle point of view cannot be imposed on the continuum, we propose a static force correction. Persistent oscillations occurring during MD-FE equilibrium indicate that the

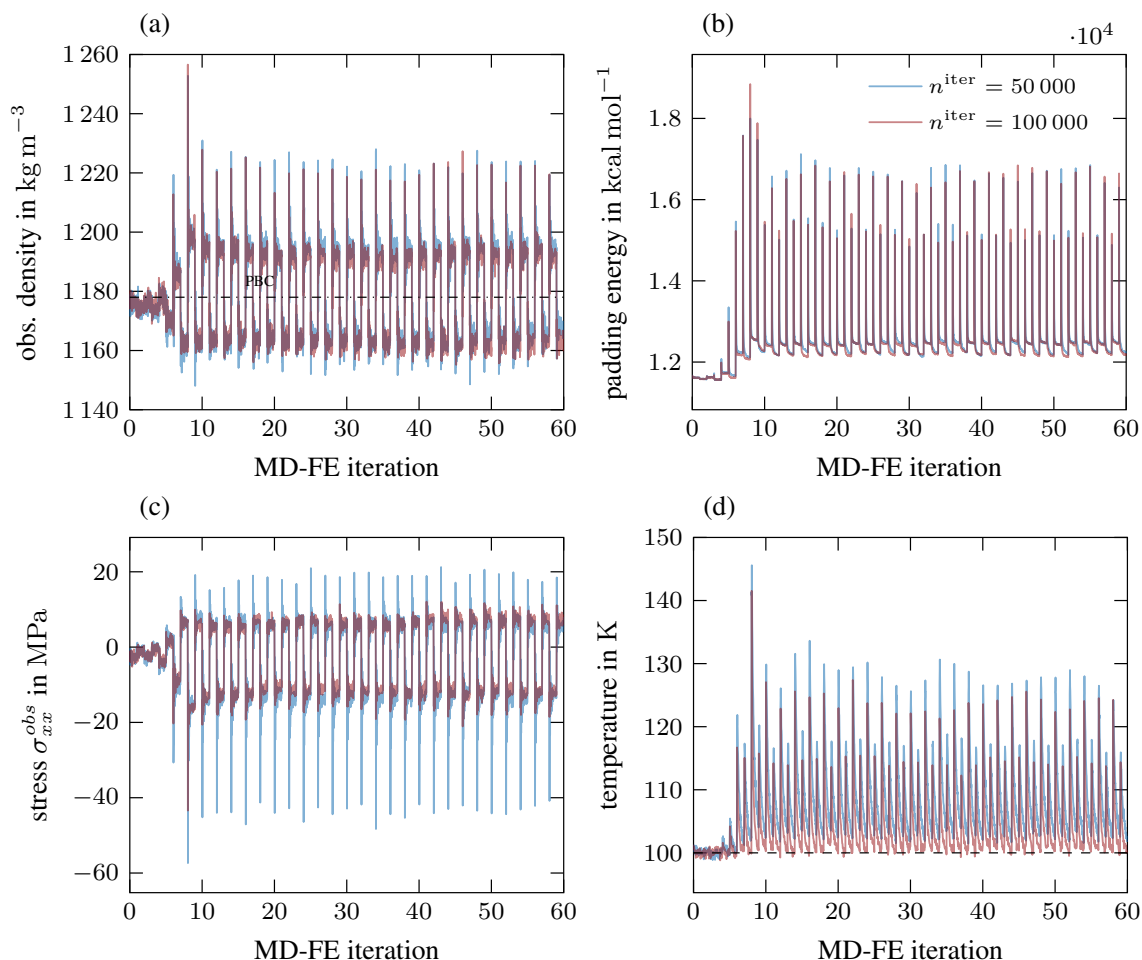


Figure 4. MD-FE equilibration: evolution of (a) density in observation region, (b) padding energy, (c) stress in observation region, and (d) temperature; PBC reference from [45].

interaction of padding atoms via MD potentials is too rigid and that the static force correction cannot cope with the dynamic behavior of amorphous polymers. This study shows that interface-based multiscale coupling for amorphous polymers poses severe difficulties. For this reason, we are currently working on incorporating a padding region into the interphase-based Capriccio method [45].

References

- [1] J. Jancar, J.F. Douglas, F.W. Starr, S.K. Kumar, P. Cassagnau, A.J. Lesser, S.S. Sternstein, and M.J. Buehler. Current issues in research on structure–property relationships in polymer nanocomposites. *Polymer*, 51(15):3321 – 3343, 2010.
- [2] Vera Bocharova, Anne-Caroline Genix, Jan-Michael Y Carrillo, Rajeev Kumar, Bobby

- Carroll, Andrew Erwin, Dmitry Voylov, Alexander Kisliuk, Yangyang Wang, Bobby G Sumpter, et al. Addition of short polymer chains mechanically reinforces glassy poly (2-vinylpyridine)–silica nanoparticle nanocomposites. *ACS Applied Nano Materials*, 3(4):3427–3438, 2020.
- [3] Jie Yang, Daniel Custer, Cho Chun Chiang, Zhaoxu Meng, and XH Yao. Understanding the mechanical and viscoelastic properties of graphene reinforced polycarbonate nanocomposites using coarse-grained molecular dynamics simulations. *Computational Materials Science*, 191:110339, 2021.
- [4] Koichi Suematsu, Masashi Arimura, Naoyuki Uchiyama, and Shingo Saita. Transparent batio₃/pmma nanocomposite films for display technologies: facile surface modification approach for batio₃ nanoparticles. *ACS Applied Nano Materials*, 1(5):2430–2437, 2018.
- [5] Zhidong Han and Alberto Fina. Thermal conductivity of carbon nanotubes and their polymer nanocomposites: A review. *Progress in polymer science*, 36(7):914–944, 2011.
- [6] Sanaz Abdolmohammadi, Samira Siyamak, Nor Azowa Ibrahim, Wan Md Zin Wan Yunus, Mohamad Zaki Ab Rahman, Susan Azizi, and Asma Fatehi. Enhancement of mechanical and thermal properties of polycaprolactone/chitosan blend by calcium carbonate nanoparticles. *International Journal of Molecular Sciences*, 13(4):4508–4522, apr 2012.
- [7] Jenny Kim, Hengxi Yang, and Peter F Green. Tailoring the refractive indices of thin film polymer metallic nanoparticle nanocomposites. *Langmuir*, 28(25):9735–9741, 2012.
- [8] Shaoyun Fu, Zheng Sun, Pei Huang, Yuanqing Li, and Ning Hu. Some basic aspects of polymer nanocomposites: A critical review. *Nano Materials Science*, 1(1):2–30, 2019.
- [9] Ali Gooneie, Stephan Schuschnigg, and Clemens Holzer. A review of multiscale computational methods in polymeric materials. *Polymers*, 9(12):16, jan 2017.
- [10] Ellad B Tadmor and Ronald E Miller. *Modeling materials: continuum, atomistic and multiscale techniques*. Cambridge University Press, 2011.
- [11] Maximilian Ries, Gunnar Possart, Paul Steinmann, and Sebastian Pfaller. Extensive CMD Simulations of Atactic PS Providing Pseudo Experimental Data to Calibrate Nonlinear Inelastic Continuum Mechanical Constitutive Laws. *Polymers*, 11(11):1824, 2019.
- [12] Maximilian Ries, Paul Steinmann, and Sebastian Pfaller. Characterization of polystyrene under shear deformation using molecular dynamics. In *Developments and Novel Approaches in Nonlinear Solid Body Mechanics*, pages 219–229. Springer, 2020.
- [13] Wuyang Zhao, Maximilian Ries, Paul Steinmann, and Sebastian Pfaller. A viscoelastic-viscoplastic constitutive model for glassy polymers informed by molecular dynamics simulations. *International Journal of Solids and Structures*, page 111071, 2021.

- [14] S. Pfaller, M. Rahimi, G. Possart, P. Steinmann, F. Müller-Plathe, and M.C. Böhm. An Arlequin-based method to couple molecular dynamics and finite element simulations of amorphous polymers and nanocomposites. *Computer Methods in Applied Mechanics and Engineering*, 260(0):109–129, 2013.
- [15] Sebastian Pfaller. Multiscale simulation of polymers, 2015.
- [16] Sebastian Pfaller, Andreas Kergaßner, and Paul Steinmann. Optimisation of the capriccio method to couple particle- and continuum-based simulations of polymers. *Multiscale Science and Engineering*, 1(4):318–333, Oct 2019.
- [17] S. Pfaller, G. Possart, P. Steinmann, M. Rahimi, F. Müller-Plathe, and M.C. Böhm. Investigation of interphase effects in silica-polystyrene nanocomposites based on a hybrid molecular-dynamics–finite-element simulation framework. *Physical Review E*, 93(5):052505, 2016.
- [18] Shengyuan Liu, Sebastian Pfaller, Mohammad Rahimi, Gunnar Possart, Paul Steinmann, Michael C. Böhm, and Florian Müller-Plathe. Uniaxial deformation of polystyrene-silica nanocomposites studied by hybrid molecular dynamics-finite element simulations. *Computational Materials Science*, 129:1 – 12, 2017.
- [19] Maximilian Ries, Gunnar Possart, Paul Steinmann, and Sebastian Pfaller. A coupled MD-FE methodology to characterize mechanical interphases in polymeric nanocomposites. *International Journal of Mechanical Sciences*, page 106564, jun 2021.
- [20] W. Zhao, P. Steinmann, and S. Pfaller. A particle-continuum coupling method for multi-scale simulations of viscoelastic-viscoplastic amorphous glassy polymers. *in preparation*, 2021.
- [21] W. Zhao and S. Pfaller. A concurrent md-fe coupling method towards simulations of fracture of thermoplastic polymers. *COMPLAS 2021, submitted*, 2021.
- [22] Sebastian Pfaller. Discrete and continuous methods for modelling and simulation of polymer materials.
- [23] Hashmi Ben Dhia and Guillaume Rateau. The Arlequin method as a flexible engineering design tool. *International Journal for Numerical Methods in Engineering*, 62(11):1442–1462, March 2005.
- [24] H. Ben Dhia, N. Elkhodja, and F. X. Roux. Multimodeling of multi-alterated structures in the Arlequin framework. solution with a domain-decomposition solver. *European Journal of Computational Mechanics*, 17:969–980, 2008.

- [25] T. Belytschko and S. P. Xiao. Coupling methods for continuum model with molecular model. *International Journal for Multiscale Computational Engineering*, 1:115–126, 2003.
- [26] P.-A. Guidault and T. Belytschko. On the l^2 and h^1 couplings for an overlapping domain decomposition method using lagrange multipliers. *International Journal for Numerical Methods in Engineering*, 70(3):322–350, April 2007.
- [27] Santiago Badia, Michael Parks, Pavel Bochev, Max Gunzburger, and Richard Lehoucq. On atomistic-to-continuum coupling by blending. *Multiscale Modeling & Simulation*, 7(1):381–406, 2008.
- [28] M. Parks, P. Bochev, and R. Lehoucq. Connecting atomistic-to-continuum coupling and domain decomposition. *Multiscale Modeling & Simulation*, 7(1):362–380, 2008.
- [29] E. B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A*, 73(6):1529–1563, 1996.
- [30] Ellad B. Tadmor. *The Quasicontinuum Method*. PhD thesis, Brown University, 1996.
- [31] Johannes J Möller, Aruna Prakash, and Erik Bitzek. FE2at—finite element informed atomistic simulations. *Modelling and Simulation in Materials Science and Engineering*, 21(5):055011, may 2013.
- [32] M. Ries, F. Weber, M. Striegel, P. Steinmann, and S. Pfaller. Multiscale FE-MD coupling: Influence of the chain length on the mechanical behavior of coarse-grained polystyrene. *Proceedings of World Congress on Computational Mechanics*, 2021.
- [33] M. Ries, P. Steinmann, and S. Pfaller. The hybrid capriccio method: A 1d study for further advancement. *Proceedings of World Congress on Computational Mechanics*, 2021.
- [34] P. J. Hoogerbrugge and J. M. V. A. Koelman. Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics. *EPL (Europhysics Letters)*, 19(3):155, 1992.
- [35] P. Español and P. Warren. Statistical mechanics of dissipative particle dynamics. *Europhysics Letters*, 30:191, 1995.
- [36] Robert D. Groot and Patrick B. Warren. Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation. *The Journal of Chemical Physics*, 107(11):4423–4435, 1997.
- [37] M. Rahimi, H. A. Karimi-Varzaneh, M. C. Böhm, F. Müller-Plathe, S. Pfaller, G. Possart, and P. Steinmann. Nonperiodic stochastic boundary conditions for molecular dynamics simulations of materials embedded into a continuum mechanics domain. *Journal of Chemical Physics*, 134:154108, 2011.

- [38] H. Qian, P. Carbone, X. Chen, H. A. Karimi-Varzaneh, and F. Müller-Plathe. Temperature-transferable coarse-grained potentials for ethylbenzene, polystyrene, and their mixtures. *Macromolecules*, 41(24):9919–9929, 2008.
- [39] Dirk Reith, Mathias Pütz, and Florian Müller-Plathe. Deriving effective mesoscale potentials from atomistic simulations. *Journal of Computational Chemistry*, 24(13):1624–1636, 2003.
- [40] H.-J. Qian, C. C. Liew, and F. Müller-Plathe. Effective control of the transport coefficients of a coarse-grained liquid and polymer models using the dissipative particle dynamics and lowe-andersen equations of motion. *Phys. Chem. Chem. Phys.*, 11:1962, 2009.
- [41] Karim Farah, Hossein A Karimi-Varzaneh, Florian Müller-Plathe, and Michael C Böhm. Reactive molecular dynamics with material-specific coarse-grained potentials: growth of polystyrene chains from styrene monomers. *The Journal of Physical Chemistry B*, 114(43):13656–13666, 2010.
- [42] Azadeh Ghanbari, Tinashe V. M. Nodoro, Frédéric Leroy, Mohammad Rahimi, Michael C. Böhm, and Florian Müller-Plathe. Interphase structure in silica-polystyrene nanocomposites: A coarse-grained molecular dynamics study. *Macromolecules*, 45(1):572–584, 2012.
- [43] M. Rahimi, I. Iriarte-Carretero, A. Ghanbari, M. C. Böhm, and F. Müller-Plathe. Mechanical behavior and interphase structure in a silica-polystyrene nanocomposite under uniaxial deformation. *Nanotechnology*, 23:305702, 2012.
- [44] Azadeh Ghanbari, Mohammad Rahimi, and Jaber Dehghany. Influence of surface grafted polymers on the polymer dynamics in a silica-polystyrene nanocomposite: A coarse-grained molecular dynamics investigation. *The Journal of Physical Chemistry C*, 117(47):25069–25076, 2013.
- [45] Y. Jain, M. Ries, F. Müller-Plathe, and S. Pfaller. Fur: An extension to the capriccio multiscale simulation method to deal with md-fe interface effects and coupling artefacts. *manuscript in preparation*, 2021.
- [46] Paul Steinmann and Kenneth Runesson. *The Catalogue of Computational Material Models: Basic Geometrically Linear Models in 1D*. Springer Nature, 2021.
- [47] Steve Plimpton. Fast parallel algorithms for short-range molecular dynamics. *Journal of computational physics*, 117(1):1–19, 1995.
- [48] MATLAB. *version 9.1.0 (R2016b)*. The MathWorks Inc., 2016.
- [49] William Humphrey, Andrew Dalke, and Klaus Schulten. VMD – Visual Molecular Dynamics. *Journal of Molecular Graphics*, 14:33–38, 1996.