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Editorial

Introduction: multi-scale modelling of radiation-induced effects in matter

Tzveta Apostolova[1,2], Jorge Kohanoff[3], Nikita Medvedev[4,5], Eduardo Oliva[3], and Antonio Rivera[3,a]

[1] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia, Bulgaria
[2] Institute for Advanced Physical Studies, New Bulgarian University, Sofia, Bulgaria
[3] Departamento de Ingeniería Energética, Instituto de Fusión Nuclear "Guillermo Velarde", Universidad Politécnica de Madrid, Madrid, Spain
[4] Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
[5] Institute of Plasma Physics, Czech Academy of Sciences, Prague, Czech Republic

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Abstract. This Topical issue collects some recent developments and specific applications of combined and multi-scale modelling in the field of intense electronic excitation of matter. It is one of the outcomes of COST Action TUMIEE (CA17126). In this introductory paper, we set the stage by discussing the paradigm of hybrid models and the motivation of development of such combined approaches.

1 Motivation

COST Action TUMIEE (CA17126) was designed to tackle the challenge of describing radiation effects in matter via multi-scale models, in particular irradiation processes that involve intense electronic excitation. Radiation effects in matter attract a lot of interest in a multidisciplinary community due to their wide variety of applications, ranging from materials processing to medical treatments. Irradiation with photons (from intense infrared beams to X-rays and gamma rays), electrons, ions, or other charged particles primarily excite the electronic component of the target material. A better understanding of phenomena induced by an intense electronic excitation would serve to advance research in a variety of fields, including solid-state physics, plasma physics, chemistry, materials engineering, computational science, electronics, photonics, medicine, geology, and astrophysics. For example, the following specific applications will benefit from progress in understanding intense electronic excitation: plume formation by intense laser irradiation [1], laser-generated particle beams [2], planet and star core studies [3], medical applications such as hadron and X-ray therapies [4], measuring of molecular structures of macromolecules and bio-particles [5], generation of high-order harmonics [6], radiation detectors [7], laser pulse diagnostic and characterization [8], materials processing with swift ions [9], creation and control of quantum dots [10], intense lasers and plasma discharges [11], materials and devices for nuclear and space environments [12], fossil dating and understanding conditions of fossil formation [13].

On the other hand, in applications using devices and materials under harsh radiation conditions, it is desirable to avoid damage as much as possible. Such applications include, e.g. bio-materials and electronics in space missions [14], plasma-wall interactions in nuclear fusion devices [15], nuclear reactor materials [16], and medical applications requiring preservation of healthy tissues during radiation treatment [17]. In those cases, it is also crucial to understand the fundamental mechanisms of material response to high energy density deposition. Advancing this understanding helps tailoring material properties to improve radiation resistance, and radiation parameters to be more benign, thus allowing for improvements in experimental and real-life applications.

From the fundamental point of view, processes of particle interaction with matter and the material response to it are still poorly understood. Classical and standard models, which are applicable to macroscopic spatial and temporal scales, fail at the ultrafast and microscopic level [18–22]. The excitation levels in the system may drive it far away from equilibrium, and induce unusual transient states of matter that exhibit unexpected behaviour [23]. Novel and innovative approaches are required to address such effects, hence motivating basic research.

High levels of electronic excitation may be produced, for example, by irradiation with conventional near-infrared to near-ultraviolet and XUV optical laser pulses, whose pulse duration may vary from atto-second

[a] e-mail: antonio.rivera@upm.es (corresponding author)

to nanoseconds, inducing different specific effects [24]. Over the past decade, it became possible to produce soft- to hard X-ray femtosecond pulses delivering a massive dose into a target in a single shot at free-electron lasers (XFEL) [5, 25, 26]. A comparable energy density may be deposited by means of swift ion irradiation [27], e.g. through laser-driven ion acceleration [28].

One of the most important advantages of femtosecond XFELs is that the pulse duration is comparable to characteristic timescales of the basic processes in solids, e.g. the typical timescales of non-equilibrium electron cascades in materials, electron–phonon coupling, particle and energy transport, etc. A spot of X-ray FEL has a typical size of one micron. The photon energy can reach up to approximately 25 keV with present-day XFELs [29], and it is expected to double in the coming years [30]. The photon attenuation length can be as short as a few tens of nanometres (for VUV at energy around the plasmon minimum), or as long as microns (for hard X-rays) [31, 32]. Thus, material modifications produced by an X-ray FEL are typically of a micron size.

Swift-heavy ions (SHI, typically with energies $E >$ 1 MeV/a.m.u.) excite primary electrons in the nanometric proximities of their trajectories. For instance, the UNILAC accelerator at GSI produces electrons with energies up to 24 keV [33, 34] by irradiation with nonrelativistic heavy ions with energies around the Bragg-peak [35]. Circular accelerators deliver even faster ions, thereby exciting electrons to higher energies. SHI impacts induce nanometric structural changes along their trajectories ranging to hundreds of microns in length, or even more [35]. The fields of optical lasers, XFEL, and SHI irradiation have many similarities (as well as peculiarities), and may mutually benefit from cross-pollination of ideas and methods [36].

Processes occurring in a target after irradiation span many orders of magnitude in space and time, which makes them intractable within a single rigorous approach. Typically, only partial aspects related to the radiation-induced effects in matter are treated. The lack of a systematic methodology to simulate the underlying phenomena hinders advances in various fields, and poses challenges to theoreticians, simulators, and experimentalists. It is therefore important to tackle this problem from a multi-scale perspective. This is precisely the realm of this Topical collection, which includes articles covering a wide range of methods, namely TDDFT, time-dependent Schrödinger equation in one- or two-electron approximation, radiation Monte Carlo, Boltzmann transport equation, radiation hydrodynamics and ab initio and classical molecular dynamics. In this collection, such mature methods and combinations of them in a multi-scale spirit are applied to the description of phenomena like laser-induced non-equilibrium electron–hole plasmas, carrier–carrier scattering, and electron–phonon coupling leading to modification and ablation of materials, plasma-based seeded X-ray lasers, high harmonic generation, electronic stopping, radioactive decay, optical energy deposition in air, formation of warm dense matter, and irradiation of interstellar ices.

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2 Characteristic scales and typical models

A number of sequential stages of material response to irradiation take place during and after ultrafast high-energy deposition into the electronic subsystem. Typical processes include the following ones:

1. Photoabsorption or energy exchange between an incident electron/ion with target electrons takes place within atto-to-femtosecond timescales. It creates primary excited electrons and leaves ionized (charged) atoms, hence driving the target out of equilibrium.
2. Initially excited electrons create secondary electrons via collisional and avalanche ionization, which typically take place at femtosecond timescale.
3. During the first ten femtoseconds [34, 37, 38], for ion or XUV irradiation, the above processes may be accompanied by Auger or radiative cascades of core holes, which are not in ionization equilibrium. Those processes generate secondary electrons or photons, whose transport proceeds in the same manner as that of primary ones.
4. The initial electronic excitation is generated in a nonthermal distribution, which evolves towards an equilibrium Fermi–Dirac distribution thermalizing via electron–electron collisions. In metals, excited electrons form an electron–hole plasma that thermalizes in a few hundred femtoseconds at temperatures considerably higher than the lattice temperature, before electrons start exchanging energy with the lattice [18, 21]. This, however, depends on the material. In semimetals like Bi, these timescales can overlap, and phonons can be excited from a non-equilibrium electronic distribution [39].
5. In semiconductors and insulators, electronic excitations lead to the formation of electron–hole pairs or excitons. Initially free, they relax into self-trapped excitons in times of the order of 100 fs. If the excitation intensity is very high, the Coulomb interaction prevents the formation of excitons, and an electron–hole plasma is formed instead. These excitations relax by exchanging energy with the lattice in quite different timescales, which can go from the sub-picosecond to hundreds of picoseconds or more for self-trapped excitons [40, 41].
6. Electrons and holes can thermalize in different timescales, which are typically much shorter than that of electron–hole recombination with photon emission. The latter happen in times of the order of nano- to micro- or even milliseconds and are responsible for luminescence phenomena such as fluorescence and phosphorescence.

7. Energy delivered to electrons may drive atoms/ions out of equilibrium too, by depositing their excess energy into the ionic subsystem and heating it (an effect of kinetic energy) or by modification of the underlying potential energy surface and hence interatomic bonding (an effect of potential energy) [36].
8. Electron–lattice (electron–phonon) coupling equilibrates the temperatures of the electron and ionic subsystems typically during a few picoseconds [18, 42–45]. The system then is in an atomically non-equilibrium state, which then may undergo solid–solid [46] or solid–liquid [47] phase transitions or even plasma formation depending on the density and distribution of the deposited energy.
9. The atomic lattice response to the heating typically occurs at pico- to nano-second timescales, ultimately cooling down in a new phase and configuration. It may also include formation of defects such as dislocations or point defects [48, 49], and macroscopic strains and stresses.
10. Macroscopic relaxation of the defected structure, such as hydrodynamic flows, structural relaxation or kinetics of defects, takes place at long, macroscopic timescales (microseconds or longer). It may result in mechanical and thermodynamic effects such as swelling or fracture, or biological effects such as cell death.

This typical example of processes taking place in a target under irradiation demonstrates that the problem of formation of observable effects spans many orders of magnitude, from atto-seconds to seconds or even longer. No single method is currently capable of tracing such a complex process.

The problem is further exacerbated by the specifics of different radiation sources and material´s kinetics. A good example is diamond—a typical material used in radiation detectors and optics. Depending on the parameters of irradiation, it may exhibit vastly different responses. Irradiated with long (pico- or nano-second) laser pulses, it may turn into graphite via atomic heating. The graphitization of this sort takes place during the corresponding pico- to nano-second timescales via *thermal* processes. That occurs at atomic temperatures above a threshold of 1600 K [50].

In contrast, irradiation with intense femtosecond laser pulses may turn diamond into graphite via *non-thermal* graphitization, which takes place via modification of interatomic potential due to excitation of electrons [51]. Nonthermal graphitization occurs within some 200 fs, long before significant energy exchange between electrons and atoms/phonons takes place [52]. This process occurs after deposition of energy of approximately 1 eV/atom into the electronic system, and practically independent on the photon energy, from infrared to X-rays [51, 53].

Yet, diamond irradiated with swift-heavy ions shows no sign of graphitization, despite vastly more energy being deposited by each ion along its trajectory [54]. All this energy is quickly brought out by excited electrons, during the extremely short time insufficient to form even nonthermal damage [36]. Very high fluences of swift ions are required to induce amorphization of diamond, occurring via accumulation of defects (which proceeds via diamond acquiring colour in shades of green).

This example illustrates that specific conditions may dramatically alter material behaviour, and appropriate models must be chosen wisely to tackle each case individually. Usually, each stage of the problem is studied separately with its own appropriate model, with shorter timescale treated with higher precision than longer ones.

The initial excitation stage (atto- to femtoseconds) may be studied with advanced *ab initio* techniques. In recent times, various methodologies have been developed and applied to study interesting phenomena such as time-dependent density-functional theory (TDDFT) [55, 56], or in femto-chemistry multi-configuration time-dependent Hartree (MCTDH) [57, 58]. TDDFT is typically combined with molecular dynamics, tracing atomic motion via the Ehrenfest approximation [59]. It is known that the electronic excitation processes are captured correctly by this approach [60], but the mean-field character of Ehrenfest distorts the characteristics of energy transfer from electrons to phonons, i.e. the Ehrenfest method cannot describe properly incoherent scattering, and hence thermalization [61]. Another difficulty in TDDFT is the exchange–correlation approximation. Most often, these are semi-local in space and local in time, or adiabatic (ALDA or AGGA), which means memory effects in the electronic evolution are ignored. This results in a lack of electronic decoherence, or in other words, electron–electron collisions are not accounted for [62, 63]. In addition, incoherent electron–phonon scattering by ionic motion (including vibrations) is not captured by TDDFT calculations [64].

To trace the electronic response to high-energy deposition, one may start from the very general equations of non-equilibrium quantum statistical mechanics, e.g. the Balescu-Resibois formalism [65] or the time-dependent non-equilibrium Green's functions approach (NEGF) [66, 67]. In the context of the intense laser irradiation of matter, these formalisms describe both coherent and incoherent interaction of electrons with sub-picosecond optical pulses, or particle irradiation, e.g. ions. Those methods are very precise, but solving the Green's function (Kadanoff–Baym) equations is computationally extremely demanding [68]. With present-day computers and algorithms, real-time NEGF methods reach timescales of only a few femtoseconds [68], while TDDFT simulations can reach the sub-picosecond regime [60], and further simplifications based on tight-binding models for the electronic structure can extend it to several picoseconds [69].

To overcome this limitation and still obtain an accurate quantum–mechanical description of the initial stages of excitation under strong electric fields

of the applied laser pulse, one can use the time-dependent Schrödinger equation (TDSE). This, however, is only feasible within a one or two active electrons approximation for the treatment of many electron systems. Combined with empirical pseudopotentials or the tight-binding method for a realistic electronic structure description, the method was successfully applied to high electronic excitation in covalent semiconductors, to obtain a prediction of ionization dynamics in diamond close to the experimental conditions necessary to produce three-dimensional conductive paths in the bulk of the substrate [70]. In addition, by calculating the deposited energy and photoelectron densities, this method describes the transient changes in the optical properties of the irradiated material in the nonlinear response regime, the threshold for excitation of surface plasmon polaritons [71], the photoexcitation of bulk plasmon [72], and the optical breakdown threshold in the bulk [73]. By calculating the ultrafast currents induced in the bulk of a material**,** one can also reliably study high harmonic generation, indicative of material structural modifications [74, 75]. This approach can be connected with the density matrix method leading to the semiconductor Bloch equations (SBE) for the time evolution of electron and hole occupations and microscopic polarization, and applied to describe interband and intraband carrier excitation, carrier dynamics, and ultrafast dephasing in semiconductors and diamond in longer timescales [76–78]. SBE can also incorporate electron–electron and electron–phonon scattering terms [79]. Electron–phonon scattering processes and electron–phonon renormalization of band structure can be computed from the lattice dynamical properties obtained from DFT or DFPT within the local density approximation (LDA) [80]. Combined with the Boltzmann or the Kadanoff–Baym equations, one can study the full dynamics in materials [41, 81]. The advantage of this method is that it is computationally less intensive than the ab initio methods described above while still incorporating the band structure of the materials ab initio, and can thus reach longer timescales.

To describe further dynamics of electrons and ions at femto- to picosecond timescales through the two-temperature stage described above, the electron–nuclear correlations need to be modelled. A possibility to do so, developed in the femto-chemistry community, is known as the "surface hopping" method [82, 83]. In this method, which is applicable mostly to molecular systems, the forces on the nuclei are determined from single electronic potential energy surfaces (PES), but electronic hops between surfaces are allowed to include non-adiabatic effects (electron transitions exchanging energy with atoms). Surface hopping works reasonably well when non-adiabatic transitions occur between a small number of PES [61], but not for a dense manifold of excited states. A method based on combining the surface hopping calculated coupling vectors (electron–ion coupling matrix elements) with Boltzmann collision integrals was recently developed and applied to solids [84, 85]. Perhaps the most sophisticated way to go beyond Ehrenfest approximation in a controlled manner is the correlated electron–ion dynamics approach (CEID) [61]. CEID relies on expansions of the quantum Liouville equation for the electron–nuclear system, with different formulations proposed in the limits of weak [86] and strong [87] electron–nuclear coupling. This approach is computationally expensive, but a more affordable variant has been proposed in the case of harmonic vibrations, i.e. electron–phonon dynamics, under the name of ECEID [88]. A re-formulation in terms of rate equations for the electronic occupations reproduced nicely the full electron–phonon dynamics at a reduced cost. This was more recently followed by a formulation of the problem purely in terms of rate equations for the coupled evolution of the electronic and phonon occupations which, in addition, includes coherences that were absent in ECEID [89].

Simplified approaches are often used to describe the two-temperature regime. They are based on kinetic models like the Master and Boltzmann equations. They are formally derived from the theory of non-equilibrium Green's functions within the framework of the quasi-particle approximation. Kinetic methods are limited to the semi-classical regime, in which electrons and holes may be treated as classical particles rather than quantum waves. Then, their dynamics is controlled by independent collisions in a Markovian process instead of coherent quantum effects [18]. Simplifications of the Liouville kinetic equation lead to the BBGKY hierarchy [90], Boltzmann's kinetic equation [91], and the Fokker–Planck equation [92]. The latter can be used to describe laser-induced dynamics in dielectrics [93, 94]. When the Markovian approximation is not fulfilled, the semi-classical approach fails and a fully quantum approach based on the evolution of the density matrix (quantum Liouville equation) should be used [79].

Kinetics of fast high-energy electrons, as well as core–hole decays, that may be well-approximated as semi-classical particles, can be traced with methods modelling individual particles instead of ensembles. They usually rely on Monte Carlo (MC) methods [95, 96]. The transport Monte Carlo method traces the propagation of individual particles, sampling occurring events with the help of random numbers. It results into a probabilistic approach, delivering statistical results such as particle and energy distributions [97]. These methods are in principle equivalent to directly solving the Boltzmann equation. However, being an integral instead of a differential method, MC can deal with non-differentiable distributions, has a reduced computational cost and is easily parallelizable. It is typically applicable at sub-picosecond timescales, until highly excited electrons relax into low-energy states that do not fall into the scope of the semi-classical approximation anymore.

To model the atomic response to the energy deposition from electrons, access to the ps-ns regime may be granted via further simplifications of the Boltzmann equation, such as hydro- or thermodynamics. Perhaps the most popular model in this category is the

two-temperature model (TTM [98, 99]), in the swift-heavy ion beam community also known as the inelastic thermal spike model. Such models, albeit easy to implement and use, do not provide sufficient detail to study material modifications and often rely on fitting parameters [100], which severely limit their applicability. A sufficient detail of the material response may be recovered with the help of classical molecular dynamics (MD) simulations [101]. Such simulations often require to additionally include an appropriate model for electron–phonon coupling, combining them, e.g. into TTM-MD [102, 103]. This has been done based on the Langevin equation, where the electronic losses are taken care of by a friction term, redistributing this energy to the atomic system via a random force [104]. In Langevin dynamics, these two terms compensate each other leading to thermal equilibration at a desired temperature. In the methodology developed by Dorothy Duffy and co-workers, the electronic degrees of freedom are represented by an electronic-temperature continuous field that is governed by a diffusion equation, while the ions are subject to the Langevin equation [105]. The latest developments in this field connect the friction coefficients to TDDFT calculations, enforcing the reproduction of the electron–phonon lifetimes computed using ground-state density-functional perturbation theory [106]. One of the limitations of this approach is that interatomic forces are generally described through a classical force field that is independent of electronic excitation. Typically, this will be an embedded atom model (EAM) for metals, a Tersoff potential for semiconductors, or a Coulomb–Buckingham potential for ionic systems (e.g. ceramics). Recently, in [47] the authors used an electronic-temperature-dependent force field based on an embedded atom model. The force field was parameterized following a methodology proposed in [107].

After the cooling of the atomic system, the target freezes into a new state, possibly with some defects formed. Those defects, such as point defects or dislocations, may further relax in the sample in longer timescales—microseconds or longer. To trace those processes, further approximate methods are employed, such as kinetic Monte Carlo (KMC) [108], which trace defect hops on the defined lattice and allow to see the dynamics of formation of experimentally observable defects aggregates, their recombination and relaxation.

If the intensity of the radiation is sufficiently high, it will generate a high density of excited electrons. These electrons ionize further electrons, developing electron cascades or avalanches [109]. This process will lead to the formation of a plasma, a quasi-neutral medium composed of electrons and charged ions (among other species). Following all the processes that take part in plasma dynamics is a complex multi-scale multi-physics problem. Propagation of intense infrared or optical laser pulses through the plasma and the interaction of its electromagnetic field with free electrons, spanning timescales from femtoseconds to tens of picoseconds or even nanoseconds, can be modelled using Particle in Cell (PIC) codes [110]. Several approximations can be applied to reduce the computational cost of the simulations and thus increase the computational domain size. For example, the paraxial and the slowly varying envelope (SVEA) approximations might be used, reducing the number an order of the partial differential equations (PDE) to solve. Other approximations take advantage of the geometry of the problem, like azimuthal decomposition in cylindrical grids.

At longer timescales (nano- to microseconds), the expansion and evolution of plasma may be described with radiative-hydrodynamic equations, enhanced with diffusive terms that model the energy transfer by electronic conduction and source/sink terms for radiative transfer. The system is completed with PDEs modelling the radiation field, whether in the diffusion approximation or solving a more accurate but complex transport equation. This leads to complex processes including mutual interaction between the plasma and the radiation field, which can be pivotal for understanding the dynamics of plasmas created inside Höhlraums. This is crucial to design and optimize inertial confinement nuclear fusion chambers as in NIF, the National Ignition Facility in LLNL [111].

As can be seen, to cover different stages (and hence different timescales) of the material response, a variety of modelling techniques is employed. To understand better the fundamental interplay of the various processes induced, and how they evolve under different experimental conditions, interdisciplinary research is needed. A cross-pollination of different fields involved should provide the necessary synergy for further breakthroughs in the science of radiation–matter interaction. This is precisely what the COST Action TUMIEE (CA17126) is all about.

3 Multi-scale models

Numerical models, combining various methods into one interconnected simulation tool, are typically known as hybrid or combined models. The idea comes from the well-established theoretical methodology of identifying parameters of the problem with respect to which approximations can be made. For example, a semi-classical free-electron approximation can be used when the kinetic energy of the electron is much greater than its potential energy of interaction, whereas a tight-binding approximation can be used in the opposite case.

However, in practical applications, we rarely deal with such clean-cut situations. Often dynamical processes in an excited electronic system drive it into a state where a part of the system, for a fraction of the time, can be approximated via free electrons, whereas another part is rather in the regime of tight binding. As mentioned in the previous section, theories applicable across multiple regimes of excitation are often unsolvable with present-day computers. Alternative approaches are thus required.

To construct a hybrid model, let us notice that the whole system may be divided into artificial subsystems, which can be described with their own efficient models. In the above-mentioned example, a fraction of excited electrons can be considered as free (a few highly energetic individual particles), whereas another fraction as tightly bound (an ensemble of strongly interacting slow particles) [21]. There is, of course, an intermediate energy region where electrons do not strictly belong to either fraction—but if this region is not highly populated, it may be neglected. Thus, a hybrid model would describe the two subsystems with their own appropriate methods and will add a proper interconnection between them.

This example demonstrates the general idea of a hybrid approach: divide and conquer. One may start with identifying the parameter space which allows for a division of the entire system into subsystems that can be described efficiently with already existing (or easily developed) models. An efficient interconnection between the models should then be constructed. Thus, the work mainly reduces to a proper description of the coupling between existing different methods.

For example, particles with very different masses, such as electrons and ions, exhibit noticeably different kinetics. This fact was used in classical approaches such as the Born–Oppenheimer (BO) approximation: electrons can be treated with quantum mechanical methods (such as DFT), whereas ions may often be traced as classical particles (within classical MD), creating a hybrid DFT-MD [112]. It also resulted into the two-temperature model (TTM), within which electrons thermalize among themselves much faster than with atoms, thereby transiently establishing two different equilibrium distributions: for electrons and for ions [98, 99, 113].

Another example is the idea to divide the processes in momentum space. It was used since the classical Boltzmann equation, in which the left-hand side described long-range fields changing a particle momentum continuously, whereas the right-hand side describes instantaneous large changes of momentum (collisions) [114]. This idea also found an application within the MC modelling approach, identifying the so-called close and distant collisions [95]. Distant collisions (with only small energy and momentum exchange) can be averaged and treated as continuous energy loss of a particle; close or head-on collisions are treated as individual scattering events. Simulation schemes that use such a separation in momentum space are called condensed history MC [95].

In a case in which different kinds of particles under consideration have different densities, they may also be described with different approximations. Dense and strongly interacting ensembles may be approximated with continuous methods (such as a kinetic equation, hydrodynamics, or a two-temperature model), while low-density ensembles of particles can be more efficiently traced individually (e.g. with Monte Carlo or molecular dynamics simulations) [115]. Another example of a combination of atomistic and continuum methods is two-temperature molecular dynamics, TTM-MD [102], discussed above.

As we saw in the previous section, a particular interest to us is to exploit the fact that the problem of materials response to irradiation consists of a set of stages separable in time. One thus may describe ultrafast effects (where an equilibrium is not reached) with non-equilibrium methods, whereas long timescales can be modelled within a thermodynamic theory, as was done, e.g. in [116, 117]. Time is a very convenient parameter to use for dividing the system and models [17, 118]. The models can often be split into independent executions and only exchange information between the two models by means of output-input files: a model without feedback [116, 117]. The problem may be divided into a large number of steps, each solvable with its own model, and interconnected into a single code tracking material response from the start of irradiation to the final experimental observable modifications [17, 119].

Similar to division in time, often systems can be divided in space due to specifics of the problem. For example, a Gaussian spatial shape of a laser beam implies that the centre of the pulse delivers much higher intensities than its tails. Even if there is damage occurring in the centre, the tails will only by slightly heated preserving the atomic structure. This suggests that the two regions in space can be described with different approaches. It has been demonstrated, e.g. that the centre may be described with an atomistic model to trace structural evolution (MD), whereas it is sufficient to describe the tails with a thermodynamic approach (TTM), tracing only the evolution of the material temperature, combined into one model, MD with TTM [120]. Methods based on division in time are more common than those implementing division in space.

Computational techniques, like adaptive mesh refinement (AMR), are particularly adapted to tackle problems with multiple spatial scales. For example, radiative hydrodynamics and laser-plasma interaction are inherently multi-scale problems. Thus, they strongly benefit from AMR. Briefly, AMR techniques refine locally the mesh in regions where a higher resolution is required to maintain a homogeneous accuracy throughout the computational domain, saving memory and computational time. This technique has been successfully applied in the field of radiative hydrodynamics for decades and, more recently, in PIC codes.

Combined models that use different methods for processes separable in space and/or time are known as "Multi-scale models" [118]. A particularly suitable and versatile multi-scale methodology [121] has been implemented in the MBN Explorer code [122] and its graphical user interface MBN Studio [123].

4 Conclusions and outlook

The field of multi-scale models is rich and quickly developing. Combinations of different models, appropriate to cover different time- and spatial scales, proved a very efficient and reliable methodology to tackle problems that are otherwise intractable. In the radiation–matter interaction, the problem spans many orders of magnitude in time: from particle scattering at the atto-second level to microseconds and the formation of observable materials modifications. Multi-scale models, combining appropriate techniques to trace each stage with necessary detail and precision, allowed in the recent years for a qualitative leap in our understanding of the fundamental processes, and thereby advanced practical applications.

This Topical issue presents the reader with some reviews of the existing state-of-the-art models, as well as with new research results obtained with them. They cover various aspects of the topic of radiation–matter interaction, in various regimes of intensities and targets.

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