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Topical Review

Future of nuclear fission theory

Michael Bender[1], Rémi Bernard[2,3], George Bertsch[4], Satoshi Chiba[5], Jacek Dobaczewski[6,7,8], Noël Dubray[3,9], Samuel A Giuliani[10], Kouichi Hagino[11], Denis Lacroix[12], Zhipan Li[13], Piotr Magierski[14], Joachim Maruhn[15], Witold Nazarewicz[16], Junchen Pei[17], Sophie Péru[3,9], Nathalie Pillet[3,9], Jørgen Randrup[18], David Regnier[3,9], Paul-Gerhard Reinhard[19], Luis M Robledo[20,21], Wouter Ryssens[22], Jhilam Sadhukhan[23,24], Guillaume Scamps[25], Nicolas Schunck[26], Cédric Simenel[2], Janusz Skalski[27], Ionel Stetcu[28], Paul Stevenson[29], Sait Umar[30], Marc Verriere[26,28], Dario Vretenar[31], Michał Warda[32] and Sven Åberg[33]

[1] IP2I Lyon, CNRS/IN2P3, Université de Lyon, Université Claude Bernard Lyon 1, F-69622 Villeurbanne, France
[2] Department of Theoretical Physics and Department of Nuclear Physics, Research School of Physics, Australian National University, Canberra, Australian Capital Territory 2601, Australia
[3] CEA, DAM, DIF, F-91297 Arpajon, France
[4] Department of Physics and Institute for Nuclear Theory, University of Washington, Seattle, Washington 98195, United States of America
[5] Tokyo Institute of Technology, 152-8550 Tokyo, Japan
[6] Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom
[7] Helsinki Institute of Physics, FI-00014, University of Helsinki, Finland
[8] Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, 02-093 Warsaw, Poland
[9] Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, Bruyères-le-Châtel, France
[10] FRIB Laboratory, Michigan State University, East Lansing, Michigan 48824, United States of America
[11] Department of Physics, Kyoto University, Kyoto 606-8502, Japan
[12] Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
[13] School of Physical Science and Technology, Southwest University, Chongqing 400715, People's Republic of China
[14] Faculty of Physics, Warsaw University of Technology, 00-662 Warsaw, Poland
[15] Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany
[16] Department of Physics and Astronomy and FRIB Laboratory, Michigan State University, East Lansing, Michigan 48824, United States of America

[17] Department of Technical Physics, School of Physics, Peking University, Beijing 100871, People's Republic of China
[18] Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States of America
[19] Institut für Theoretische Physik II, Universität Erlangen-Nürnberg, 91058 Erlangen, Germany
[20] Center for Computational Simulation, Universidad Politécnica de Madrid, E-28660 Madrid, Spain
[21] Departamento de Física Teórica and CIAFF, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
[22] Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520, United States of America
[23] Variable Energy Cyclotron Centre, Kolkata 700064, India
[24] Homi Bhabha National Institute, Mumbai 400094, India
[25] Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine CP 226, BE-1050 Brussels, Belgium
[26] Nuclear and Chemical Science Division, Lawrence Livermore National Laboratory, Livermore, California 94551, United States of America
[27] National Center for Nuclear Research, Pasteura 7, 02-093 Warsaw, Poland
[28] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, United States of America
[29] Department of Physics, University of Surrey, Guildford, Surrey, GU2 7XH, United Kingdom
[30] Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, United States of America
[31] Department of Physics, Faculty of Science, University of Zagreb, Croatia
[32] Institute of Physics, Maria Curie-Skłodowska University, 20-031 Lublin, Poland
[33] Mathematical Physics, Lund University, S-221 00 Lund, Sweden

E-mail: jacek.dobaczewski@york.ac.uk

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Abstract

There has been much recent interest in nuclear fission, due in part to a new appreciation of its relevance to astrophysics, stability of superheavy elements, and fundamental theory of neutrino interactions. At the same time, there have been important developments on a conceptual and computational level for the theory. The promising new theoretical avenues were the subject of a workshop held at the University of York in October 2019; this report summarises its findings and recommendations.

Keywords: nuclear fission, nuclear theory, spontaneous fission, induced fission

(Some figures may appear in colour only in the online journal)

1. Introduction

The theory of nuclear fission has a long history, driven for many years by technological applications and heavy element studies. Today the needs are even broader with the recognition of new connections to other disciplines such as astrophysics and fundamental science.

In the past, fission theory was largely phenomenological. Recent significant advances in microscopic modelling, which can be tested thanks to the rapid growth in computational capabilities including leadership-class computers, provide opportunities for developing fission theory to a new level of refinement. In addition, experimental fission data of unprecedented detail and quality are now being acquired and can be used to validate models more thoroughly.

A disclaimer is in order, because we used the word 'microscopic' in the previous paragraph. In the context of fission theory and indeed all theory that is applied to large nuclei, 'microscopic' should not be construed as an *ab initio* many-body theory with all Hamiltonian input taken from the outside. In our field, theory is useful at a quantitative level only if the parameters, or coupling constants, of models are optimised to experiment. For that reason, all quantitative nuclear models are phenomenological at some level. Superlatives such as 'fully microscopic' or 'from first principles', sometimes used to characterise particular approaches, may be viewed more as wishful thinking than the present reality. However, it is useful to distinguish the degrees of phenomenology in different theoretical approaches. In this document we will use the term 'microscopic theory' for theoretical approaches in which nucleonic degrees of freedom are explicitly present together with inter-nucleon forces. The most prominent example is nuclear density functional theory (DFT) which is based on effective nucleon–nucleon interactions that generate mean fields and the associated single-particle orbitals. In this document we assess the future promise of a number of extensions of DFT. Some of them remain microscopic, but others are best characterised as phenomenological.

This document was initiated at the Workshop on *Future of Theory in Fission* held in York in October 2019 (https://www.york.ac.uk/physics/news/events/groups/nuclear-physics/2019/future-of-theory-in-fission-workshop/). The premise of the meeting was that fission theory is ripe for rapid progress. Consequently, the focus was on future developments, perspectives, and challenges. The questions motivating the workshop were:

- Considering the broad range of observables, what are the physics objectives that fission theory needs to address?
- What are realistic goals that can be achieved with advanced microscopic frameworks and modern computational tools?
- Can microscopic theory provide justification for successful phenomenological assumptions and models?
- Which current approximations routinely made in fission studies are justified or not, or unavoidable or not, in view of the present-day computational capabilities? What are the robust approximations that can be employed to simplify the treatment and/or reduce the computational effort?
- Is it realistic to envision a unified microscopic theory of fission that would cover the entire energy range from spontaneous fission (SF) to fission well above the barrier?
- What are the best strategies for the community to optimise fission theory research?

As seen from the list of sections, this document summarises the broad range of topics covered in the York Workshop. Our unifying theme is the pathway towards solving the fission

problem via modern many-body frameworks by taking advantage of the latest computational methodologies. In this context, the main purpose of this document is to outline challenges and point to possible solutions rather than to provide a detailed review of nuclear fission theory. The interested reader is encouraged to consult recent reviews of various aspects of fission theory, e.g., Schunck and Robledo (2016) (overview of microscopic models) and Andreyev *et al* (2017), Talou *et al* (2018), Schmidt and Jurado (2018) (description of state-of-the-art fission phenomenology), which contain extensive lists of references.

Of the various shape regions depicted in figure 1, we shall cover microscopic dynamics in the domains around the initial state and the barriers as well as the highly deformed region beyond. But we are leaving out the important challenge of describing how the system propagates from one region to another because there has been virtually no coherent microscopic theory addressing this question up to now. This underscores the fact that there will still be much future work to do in nuclear fission theory.

2. Main features of fission

To set the stage for the subsequent specialised considerations, we begin with a brief presentation of the main features of the nuclear fission phenomenon. Figures 1 and 2 present schematic illustrations of the evolution leading from a single nucleus to two pre-fragments, nascent fragments, primary fragments, which subsequently appear in detectors as fission fragments, see caption of figure 2.

Fission is a time-dependent transformation which can be conveniently separated into distinct stages, each characterised by its own time scale, as shown in figure 2. The process proceeds from some initial state through a complicated collective evolution ending with the emergence of two excited nascent fragments. They in turn undergo a sequence of prompt and/or delayed de-excitations decays ending with two product nuclei in their ground or isomeric excited states[35].

The most obvious physical attribute during the evolution of the fissioning nucleus is its overall elongation, correlated with the different stages as shown in figure 1. Initially the elongation is that of the equilibrium shape of the mother nucleus. From this, the collective evolution proceeds through a sequence of shapes whose time-dependent elongations exhibit a diffusive behaviour. Eventually the system finds itself beyond the outer saddle point and then evolves towards scission, as its shape takes on a binary form and the elongation grows ever larger. At scission the system divides into nascent fragments which are then accelerated apart.

2.1. Spontaneous and induced fission

It is useful to distinguish SF which occurs in nuclei in their ground states from induced fission brought about by a reaction or decay process bringing in energy from the outside. SF is one of the main decay modes of superheavy nuclei and is therefore of great interest in the experimental search for them. While SF primarily occurs from the nuclear ground state, it has also been observed from isomeric states.

On the theory side, the relatively long lifetimes are due to the existence of a potential barrier that must be penetrated. Consequently SF is an inherently quantal process; see section 3.6. An interesting aspect of SF is its dependence on the number parity of the nucleus: in odd–A nuclei it is typically hindered by $\sim$ 3–5 orders of magnitude relative to their even–even neighbours. Fission of odd–odd nuclei is believed to be even more hindered, but credible data are scarce.

[35] In this paper, we are not concerned with the extremely rare phenomena of ternary and quaternary fission.

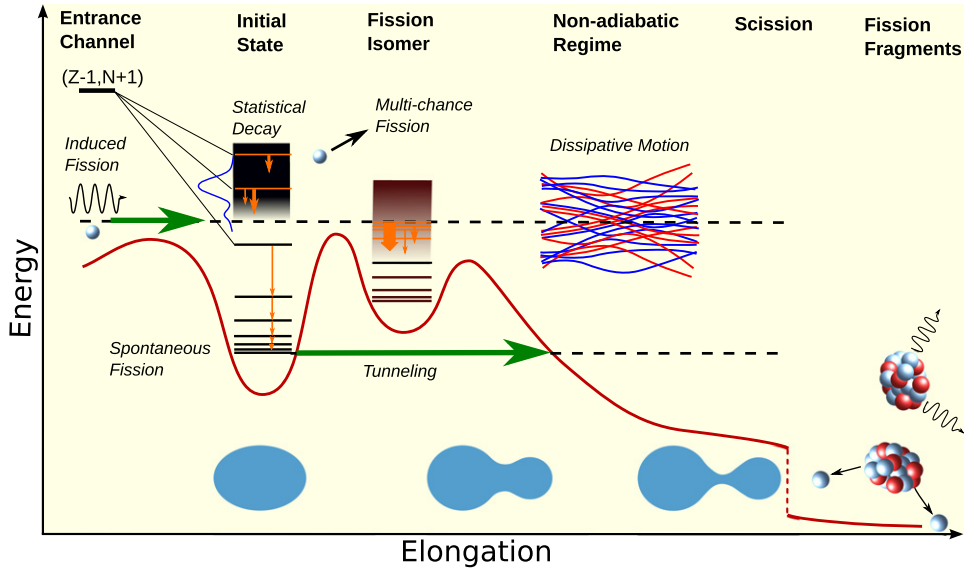

Figure 1. Schematic illustration of the features most relevant to the fission phenomenon. The red curve depicts (in a one-dimensional projection) the potential energy as a function of the elongation; the ground state is at the lowest minimum, and the shape-isomeric state is at the second minimum. From these states it is possible to tunnel through the potential barrier. Tunnelling is also relevant for neutron or photon induced fission when the resulting initial state lies below the fission barrier. If the initial state is excited above the fission barrier, it may undergo a complicated shape evolution crossing the barrier from above. Once the system finds itself beyond the barrier, it relatively quickly descends towards scission. There it divides into two nascent fragments, which subsequently move apart under the influence of their mutual Coulomb repulsion while gradually attaining their equilibrium shapes and become primary fragments. Primary fragments then de-excite by evaporating neutrons, radiating photons, and undergoing β decay.

In addition to an SF, fission can be induced by a variety of nuclear reactions. The fission-induced processes include: neutron capture (responsible for energy production in fission reactors), electron capture and beta decay, photofission, and reactions involving charged particles and heavy ions. In all these processes, the fissioning nucleus is created in an excited state, which may lie above or below the fission barrier.

Theoretical descriptions of fission induced by fast probes often assume the creation of a compound nucleus at a given thermal excitation energy. However, as discussed later, that assumption might be ill-founded for fast probes because the nuclear system may not have sufficient time to thermalise before undergoing fission. This becomes increasingly important at higher energies where pre-equilibrium processes play an increasingly significant role and may lead to the emission of one or more nucleons before equilibrium is reached. Moreover, as the excitation energy of the compound nucleus is increased, neutron evaporation competes ever more favourably with fission and as a result, one or more neutrons may be evaporated before fission occurs (multi-chance fission). In addition, for non-thermalised systems one should develop approaches using fixed energy rather than fixed temperature.

2.2. Important observables

When talking about fission observables, it is important to remember that what is often considered ‘experimental’ is often the result of an indirect process, in which a quantity of

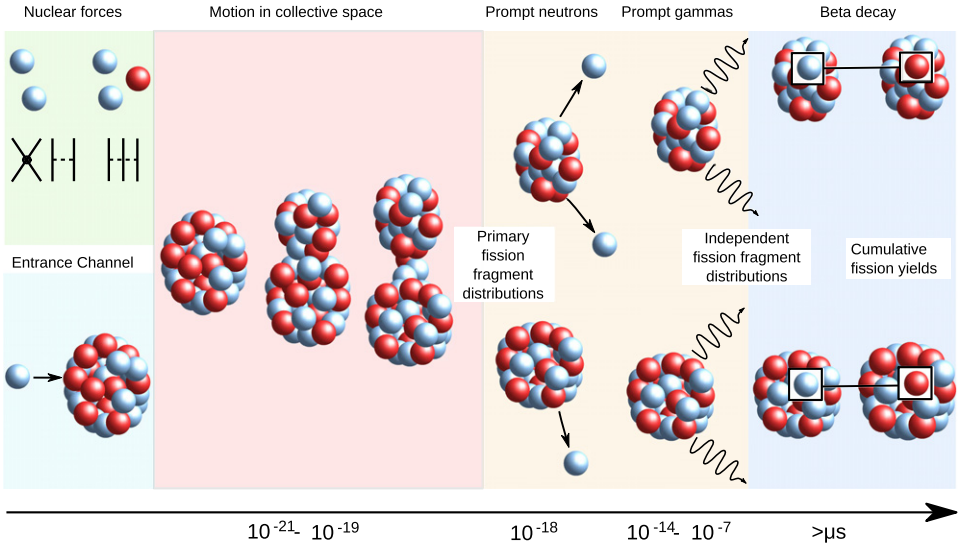

Figure 2. Schematic representation of the different stages of a fission process, starting from the initial nucleus (on the left), approaching the scission point as pre-fragments, dividing into two excited nascent fragments, which after getting fully Coulomb accelerated become primary fragments, then promptly emit neutrons and photons and undergo β decays, and finally become fission fragments in the exit channel. The associated time scales are indicated on the axis underneath.

interest is extracted from measurements with the help of some model or model-dependent assumptions.

Nuclear fission is a very complex transformation and there are many quantities of interest that are directly measurable and subject to theoretical modelling. [A set of key fission observables suitable for validation of theoretical models was proposed in Bertsch *et al* (2015).] We list here some of the most important ones, with their common designations:

Spontaneous-fission half-lives (T_{SF}). Measured SF lifetimes (or half-lives) span a range from microseconds or smaller to billions of years. To describe such a range is a significant challenge to theory.

Total and differential fission cross sections. For instance, the neutron induced fission cross section σ(n, f) and its energy and angular dependence or the threshold energy for fission observed in a photo-fission cross section that is closely related to the height of a fission barrier.

Yields ($Y(A)$, $Y(Z)$, $Y(Z,A)$). They describe probabilities for producing fission fragments of given mass and/or charge. Such data are particularly important in nuclear astrophysics. Yields refer to primary, independent or cumulative distributions (see figure 2).

Fission spectrum. This includes the average number of neutrons per fragment, their energies, the average number of photons per fragment and their energies, multiplicity distributions, angular correlations, etc.

Total kinetic energy (TKE). The post-acceleration kinetic energy of the fission fragments, its distribution, and its dependence on fragment mass.

Beta-decay spectrum of fission products. This is particularly important for the fundamental theory of beta decay and includes the neutrino spectrum.

Correlations between the above quantities (e.g., between fragment mass and TKE), as well as with other quantities (e.g., with the spin of the fissioning nucleus) are also very important. We wish to emphasise that the fission observables should be accompanied by uncertainties. This is crucial in the context of nuclear data evaluation and applications in general.

In this context, it is useful to mention some important unobservables (physical concepts that cannot be observed directly). Arguably, the most celebrated quantity that belongs to this group is the fission barrier. Fission barrier height can be defined theoretically as the energy difference between the ground state and the highest saddle point in a computed potential energy surface (PES) that has the lowest energy for all possible paths leading to fission from the ground state. Fission barriers inferred from measured cross sections are plagued with ambiguities because the extraction procedure is often based on a simplistic picture of a fission pathway. Another unobservable concept is that of a compound nucleus; it is based on a model that assumes the full thermalisation of the system and ignores pre-equilibrium processes. Other useful yet unobservable quantities include: scission point at which the nucleus breaks into nascent fragments, shell energy on the path to fission, pairing energy at the barrier, and pre-fragments that are formed in the pre-scission region.

3. Basic concepts of fission theory

To lay the groundwork for discussing the promising ideas for future development, we recall here some of the basic theoretical tools at our disposal. In time-dependent formalisms, basic distinctions can be made between dynamics based on inertial motion, dynamics based on diffusion motion in a statistical framework, and dynamics that combine inertial and diffusive motion. The relevant computational methodologies are often referred to by their acronyms; the ones used here are listed in table 1.

Before going into details of different concepts discussed below, we want to touch upon one specific term that is abundantly used in the theory of nuclear fission, namely, the concept of adiabaticity. First, a disclaimer is in order, because in the rigorous (electronic) time-dependent DFT (TDDFT), see, e.g. Burke *et al* (2005), the term 'adiabatic' has a different meaning than here. Indeed, there it denotes an approximation of the time-dependent functional that is local in time and thus disregards memory effects. In this sense, all time-dependent approaches to fission, which we discuss below, are adiabatic, and releasing this constraint in nuclear physics probably belongs to the future not covered by the present report at all.

In nuclear physics, the term 'adiabatic' has several interwoven, although not fully identical facets. First, it may mean that the collective motion proceeds through a sequence of local ground states, each corresponding to the system being constrained to a given set of collective coordinates and intrinsic quantum numbers. Adiabatic motion then means that a time-dependent wave function acquires collective kinetic energy through infinitesimal admixtures of local excited states, whereas non-adiabatic corrections correspond to significant admixtures of those. A dissipative motion (section 3.5) means a constant irreversible flow of energy away from the local ground state.

Provided the local ground states are well defined and do not cross with excited states, this constitutes a coherent physical picture. However, this picture breaks down in situations where several local ground states (characterized by different intrinsic quantum numbers) coexist and compete energetically (e.g., different one-quasiparticle states in odd–A nuclei). Then, the system may proceed diabatically, along a fixed configuration, or adiabatically, by changing the configuration, depending on the Landau–Zener probability of a diabatic transition (section 3.7).

Table 1. Glossary of used acronyms pertaining to nuclear fission models and fission characteristics (in alphabetic order).

Acronym	Meaning
ATDDFT	Adiabatic TDDFT
ATDHFB	Adiabatic TDHFB
BCS	Bardeen–Cooper–Schrieffer
CHF	Constrained HF
CHFB	Constrained HFB
CSE	Collective Schrödinger equation
DDD	Dissipative diabatic dynamics
DFT	Density functional theory
EDF	Energy density functional
GCM	Generator coordinate method
GOA	Gaussian overlap approximation
HF	Hartree–Fock
HFB	Hartree–Fock–Bogoliubov
HO	Harmonic oscillator
MM	Microscopic macroscopic
PES	Potential energy surface
QRPA	Quasiparticle RPA
RPA	Random phase approximation
SF	Spontaneous fission
TDDFT	Time-dependent DFT
TDGCM	Time-dependent GCM
TDHF	Time-dependent HF
TDHFB	Time-dependent HFB
TDRPA	Time-dependent RPA
TKE	Total kinetic energy

In the context of the time-dependent Hartree–Fock (TDHF) or TDDFT, adiabaticity denotes a very specific approximation of the time-dependent one-body density matrix, which is assumed to have the time-odd part much smaller than its time-even part (Baranger and Véneroni 1978). In essence, this approximation holds only when the motion is appropriately slow. Another commonly used definition of adiabaticity involves a separation of variables into slow and fast coordinates (Tully 2012). Many concepts of fission theory, such as the collective Schrödinger equation (CSE), are based on the division of degrees of freedom into 'collective' and 'non-collective'.

All those definitions are connected by the fact that, in practice, the local ground states can only be considered within the mean-field picture, which means the TDDFT interpretation of the one-body evolution. A weak mixing with low-lying excited states is then equivalent to the requirement of the slow motion. In the following, the notions of adiabaticity and dissipation are discussed in many places, as undoubtedly they constitute pivotal points of the theoretical description of fission.

3.1. Time scales

It is important to understand the various time scales associated with the different stages of fission in order to anticipate the kind of dynamics that would be needed in the theory. One of the most intriguing questions about fission dynamics is the time it takes for fission to occur.

There are in fact several time scales that affect the duration of the fission process. Fission that goes through the compound nucleus is delayed by the compound nucleus lifetime, which is much longer than the dynamics time scales. At excitation energies below the fission barrier, the fission lifetime is largely dominated by the tunnelling probability and can vary by many orders of magnitude. The next scale is that of the collective motion from the outer turning point to scission, see figure 1. The slower this is, the more valid will be diffusive and statistical modelling of the dynamics. Finally, the time it takes to scission plays a special role affecting particularly the TKE and excitation energies of the fragments. At higher energies, the distinctions between the different stages are less clear, but the basic dynamics taking the system from a highly excited compound nucleus to a scission configuration is governed by a similar time scale.

One of the most difficult questions to investigate experimentally is fission time scales since they involve the early stages of fission dynamics. They are not generally accessible directly but must be inferred from the analysis of products at later stages of fission. Experiments attempting to measure fission times (Hinde 1993, Jacquet and Morjean 2009, Frégeau *et al* 2012, Sikdar *et al* 2018) often need to be complemented by a model description of, e.g., the emitted neutrons and their dependency on angular momentum or excitation energy. See section 7.7 for a discussion of this topic. As a result, it is likely that different experimental methods probe different characteristics of the fission time distribution. Theoretically, in addition to dynamics, statistical processes such as particle emission and thermal fluctuations may be important. In general, one needs theoretical approaches accounting for fluctuations in order to predict the entire fission time distribution instead of the average or most likely time.

3.2. Mean-field theory

The mean-field approximation provides the backbone of microscopic nuclear theory for all but the lightest nuclei. In the context of nuclear fission, the great advantage of the mean-field theory is that it is directly formulated in the intrinsic, body-fixed reference frame of the nucleus, in which the concept of deformed nuclear shape and its dynamical evolution is naturally present.

Briefly, the self-consistent many-body wave functions are directly or indirectly composed of Slater determinants of orbitals, with the orbitals computed as eigenstates of one-body mean-field potential. If the mean-field potential is determined by the expectation value of a Hamiltonian in the Slater determinant, we arrive at Hartree–Fock (HF) approximation. If a pairing field is included, we arrive at the Hartree–Fock–Bogoliubov (HFB) approximation. As in electron DFT of condensed matter and atomic physics, the Fock-space Hamiltonian is often replaced by an energy density functional (EDF) defined through one-body densities or density matrices. As is common practice in the nuclear physics literature, we will use these notions interchangeably, where HFB and HF are used to distinguish between nuclear DFT with (HFB) and without (HF) treatment of pairing correlations. The use of an EDF instead of a Hamilton operator sometimes necessitates to take different intermediate steps in formal derivations, but leads to self-consistent equations that for all practical purposes coincide with those of HF (or HFB if pairing is present).

Another approach in common use, the macroscopic–microscopic (MM) method, avoids the delicate issues of constructing an EDF that reproduces the systematic properties of heavy nuclei. Here the basic properties of the nucleus are derived from its size and shape, expressed in some parameterisation of the surface. The orbitals are constructed with a potential derived from the shape of the nuclear surface, and its energy is computed using the liquid drop model together with shell corrections determined by the orbital energies. The first quantitative theoretical understanding of fission came from this approach (Brack *et al* 1972, Bjørnholm and

Lynn 1980), see also its review in Krappe and Pomorski (2012), and it has been successfully applied to calculate mass and charge yields.

In HF and HFB, wave functions representing different nuclear shapes are constructed by constraining the single-particle density matrix in some way. This is often implemented by adding fields with Lagrange multipliers, but it can also be done more directly; see section 8.1.2. Typically, in nuclear DFT the nuclear shape is defined by several parameters that are taken as collective variables.

3.2.1. Potential energy surface. The PES represents the lowest possible energy of the evolving system consistent with the specified values of the collective variables. As mentioned above, the PES is generally multi-dimensional. Although the PES alone does not suffice for predicting the dynamical evolution, it is nevertheless very useful because its topography makes it possible to understand and anticipate the main features of the dynamics. The local minima, saddle points, and the scission surface are key features that often make it possible to predict isomeric properties, threshold energies, and fission fragment yields.

For a given point in the collective space, the potential energy of the corresponding nuclear configuration and its internal structure can be obtained either by minimising the total energy in the CHF (constrained HF) or CHFB (constrained HFB) framework or by calculating the MM energy for the specified shape. The first method results in an optimised shape within the given constraints while the second method can miss aspects of the shape beyond the defined shape parameterisation. There are important consequences in both methods for defining the collective space variables and for the continuity of the resulting surface (Möller *et al* 2001, Dubray and Regnier 2012, Schunck *et al* 2014).

While the standard PES describes the configuration having no excited orbitals or quasiparticle excitations, some approaches need energy in the presence of internal excitations. In the MM method it requires the calculation of shell and pairing corrections at finite excitation (Ignatyuk *et al* 1980), while the self-consistent method may employ a temperature-dependent DFT formalism (Egido *et al* 2000, Pei *et al* 2009, Sheikh *et al* 2009, Schunck *et al* 2015a, Zhu and Pei 2016).

3.2.2. Other constraints in DFT. The PES is usually presented as a function of a few multipole moments in the CHF and CHFB framework, but multipole moments control the shape only loosely and do not provide sufficient discrimination between intrinsic configurations at large elongations. When needed, other types of constraints can provide additional discrimination power. For example one can define a neck-size parameter to be added to the multipole moments (Warda *et al* 2002). More drastically, the entire density distribution $\rho(\boldsymbol{r})$ can be constrained. Such a density-constrained method (Cusson *et al* 1985, Umar *et al* 1985) has been used successfully within TDHF (time-dependent HF) approach to calculate heavy-ion interaction potentials (Umar and Oberacker 2006, Simenel and Umar 2018). For a sequence of shapes in the collision, the instantaneous density of the evolving system obtained in TDHF is used as a constraint for a static HF calculation, yielding the lowest-energy configuration compatible with the constraint. This eliminates both the collective kinetic energy and the internal excitation and may therefore be interpreted as the potential energy. While this information is important for going beyond TDHF and TDHFB (time-dependent HFB), there is no simplification in the dynamics when taking the r-dependent density as a collective variable. See section 4.1 for additional discussion of collective variables.

It is also possible to introduce constraints that depend more on the wave function than on the shape. In particular, one can get a high discriminatory power in the space of axially symmetric configurations by requiring a certain filling of the orbitals with respect to their axial symmetry

(Bertsch *et al* 2018). See also constraints pertaining to the strengths of pairing correlations, discussed in section 4.1.

3.3. Time-dependent DFT

The time-dependent version of HF is an established approach to nuclear dynamics and has been extensively used to model heavy ion collisions (Simenel 2012, Simenel and Umar 2018, Sekizawa 2019). In principle it can be easily generalised to the HFB approximation, but one is only now reaching the computational power to carry out calculations without introducing artificial constraints and approximations (Bulgac *et al* 2016, Hashimoto and Scamps 2016, Scamps and Hashimoto 2017, Magierski *et al* 2017, Bulgac *et al* 2019a). These approaches have an important property that they respect energy conservation and the expectation values of conserved one-body observables such as particle number. Their strong point is that they usually give a good description of the average behaviour of the system under study. Their weak point is that, since TDHF equations emerge as a classical field theory for interacting single-particle fields (Kerman and Koonin 1976), the TDDFT approach can neither describe the motion of the system in classically-forbidden part of the collective space nor quantum fluctuations. As a consequence, the real-time TD approach cannot be applied to SF theory. Moreover, the fluctuations in the final state observables, some being due to non-Newtonian trajectories (Aritomo *et al* 2014, Sadhukhan *et al* 2017), are often greatly underestimated in time-dependent approaches.

3.4. Beyond mean-field theory

While the symmetry-broken product wave function of HFB already provides a very good description for many properties, it is deficient if a self-consistent mean-field symmetry is weakly broken. In such cases, it is advisable to extend the method beyond a single-reference DFT. One way of doing this is to use the small amplitude approximation to the TDHFB, i.e., the quasiparticle random phase approximation (QRPA). The QRPA is a *vertical* expansion that accounts for selected correlations coming from excited states of the system. Another way of enriching the DFT product state is through a multi-reference DFT (Bender *et al* 2019). This represents a *horizontal* expansion (Dönau *et al* 1989). Two commonly used beyond-DFT methods belong to this category. One is the generator coordinate method (GCM). The GCM wave function is a superposition of single-reference DFT states computed along a collective coordinate (or coordinates). The second group contains various projection techniques, in which the projection operation is applied to an HFB state in order to restore internally-broken symmetries. The most advanced multi-reference DFT approaches combine the virtues of the vertical and horizontal expansion by employing the GCM based on the projected HFB states, which often contain contributions from multi-quasiparticle excitations.

3.4.1. Generator coordinate method. A microscopic Hamiltonian treated in the CHF or CHFB approximations can be mapped onto a CSE in the coordinates defined by constraints. This mapping is the essence of the GCM. Typically the mapping is carried out using the Gaussian overlap approximation (GOA) to determine the kinetic energy operator. Examples of such calculations for low-energy fission can be found in Goutte *et al* (2004), Goutte *et al* (2005), Erler *et al* (2012b), Regnier *et al* (2016), Zdeb *et al* (2017), Tao *et al* (2017), Regnier *et al* (2019), Zhao *et al* (2019). With several coordinates, the GCM produces much wider distribution in the mass yields than can be realised in the evolution in time of a single CHF or CHFB configuration. On the other hand, the underlying wave function is composed of zero-quasiparticle configurations and so underestimates the non-collective internal energy.

To take into account non-adiabatic effects during the fission process, the inclusion of excitations built on the zero-quasiparticle vacuum becomes essential. Several experimental observables attest to the importance of two-quasiparticle (2-qp) excitations, which include the pair-breaking mechanism and the coupling of pairs to the collective degrees of freedom. From this point of view, the inclusion of explicit 2-qp components into the GCM wave function is of interest (Bernard *et al* 2011). One of the major advantages of the model is the nonlocal nature of the couplings between collective modes and intrinsic excitations. The development of this approach, however, poses several problems related to the truncation of the 2-qp space; keeping track of excitations along the collective path; and evaluation of overlap kernels. So far, the model presented in Bernard *et al* (2011) has not yet been be applied to fission problems.

3.4.2. Projection techniques. The nuclear Hamiltonian commutes with particle number, angular momentum, and parity symmetry operations. The density functional of nuclear DFT is usually symmetry-covariant (Carlsson *et al* 2008, Rohoziński *et al* 2010). Still, due to the spontaneous breaking of intrinsic symmetries in mean-field theory, several symmetries are usually broken in a nuclear DFT-modeling of fission. There are well-established projection methods to restore broken symmetries based on the generalised Wick's theorem (Mang 1975, Stoitsov *et al* 2007, Bender *et al* 2019, Sheikh *et al* 2019) that have been applied to calculations of the fission barrier of ^{240}Pu, either combining parity and particle-number projection (Samyn *et al* 2005), or combining angular-momentum and particle-number projection with shape mixing (Bender *et al* 2004). The methods are straightforward in principle for models based on a Fock-space Hamiltonian. Difficulties can arise in EDF realisations of nuclear DFT, as discussed in Anguiano *et al* (2001), Dobaczewski *et al* (2007), Bender *et al* (2009), Duguet *et al* (2009), Sheikh *et al* (2019)). However, these problems do not concern the calculation of one-body observables such as the average particle number in the fission fragments (Regnier and Lacroix 2019, Bulgac 2019).

3.5. Dissipative dynamics

While the self-consistent DFT dynamics is very powerful, it largely ignores the internal degrees of freedom that can bring large fluctuations of observables and dissipate energy (Kubo 1966, Yamada and Ikeda 2012). There are several ways that the additional degrees of freedom can be taken into account in the equation of motion.

A simple diffusion master equation assumes the presence of first-order time derivatives. This approach has been remarkably successful in describing mass and charge yields (Randrup and Möller 2011). While the utility of this ansatz has received some support from recent microscopic calculations (Bulgac *et al* 2019a), its quantitative validity still needs to be derived.

More generally, one can consider time-dependent models that combine time-even inertial dynamics with time-odd dissipative dynamics. A common classical formulation is with a multi-dimensional Langevin equation (Sierk 2017, Usang *et al* 2019). In this approach, the dissipated energy goes into a heat reservoir characterised by a temperature. Recently, a hybrid Langevin-DFT approach has been applied to explain SF yields (Sadhukhan *et al* 2016). While this is reasonable in a phenomenological theory, there is so far no microscopic justification of this approach. It is to be noted, however, that the predicted fission yield distributions are found insensitive to large variations of dissipation tensor (Randrup *et al* 2011, Sadhukhan *et al* 2016, Sierk 2017, Matheson *et al* 2019). The corresponding quantum dynamics requires an equation of motion for the density matrix of the system. One formulation is with the Lindblad equation; see also Bulgac *et al* (2019b).

3.6. Quantum tunnelling

Tunnelling motion in SF is usually treated via a quasiclassical, one-dimensional formula for the action integral which is based on two main quantities that can be obtained in nuclear DFT: the PES and the collective inertia (or mass) tensor. The fission path is computed in a reduced multidimensional space, using between two and five collective coordinates describing the nuclear shape and pairing; see section 4.1. The mass tensor requires the assumption of a slow, near-adiabatic motion; see section 4.2. The pairing gap makes this assumption most credible for even–even nuclei, but even in such systems one can expect non-adiabatic effects due to level crossings (Schütte and Wilets 1975a, Schütte and Wilets 1975b, Strutinsky 1977, Nazarewicz 1993). The following questions are relevant for making progress in SF studies.

Generalised fission paths. Usually, SF trajectories in the collective space are determined by considering several shape-constraining coordinates. It is better to assume that the collective motion happens in a large space parameterised by the Thouless matrix characterising an HFB state. One approach to determine the collective path in that way has been proposed in Marumori *et al* (1980) and Matsuo *et al* (2000). There the equations of motion have a canonical form (involving both coordinates and momenta), and constraining operators are dynamically determined.

Multi-dimensional WKB formula. The current barrier-penetration methodology is based on a minimisation of the collective action along one-dimensional paths, although our experience with above-barrier fission evolution suggest that the use of several degrees of freedom is important. It may be possible to generalise the one-dimensional quasiclassical WKB-like formula by a more general solution to a few-dimensional tunnelling problem (Scamps and Hagino 2015).

Non-adiabatic effects. The admixtures of non-adiabatic states may be crucial to understand fission hindrance in odd nuclei. The excitations to higher configurations can be induced by crossings of single-particle levels and by the Coriolis coupling; see section 3.7.

Instanton formalism. An alternative approach is provided by the formalism of imaginary-time TDHFB (Reinhardt 1979, Levit *et al* 1980, Puddu and Negele 1987, Negele 1989, Skalski 2008). Configuration mixing can be performed according to well defined equations, and SF lifetimes could be determined without having to define collective inertia. Non-self-consistent solutions using a phenomenological Woods–Saxon potential and omitting pairing have already been obtained (Brodziński *et al* 2018). If the simplified approach with pairing gives the proper order of magnitude for the fission hindrance and its weak dependence on particle numbers, the next step would be to incorporate the requirement of self-consistency.

3.7. Level crossing dynamics

In the original framework for a microscopic theory of fission above the fission barrier, Hill and Wheeler (Hill and Wheeler 1953) proposed a model based on time-dependent diabatic evolution of mean-field configurations interrupted by possible jumps to other configurations at the points of level crossings. At those intersections the probability to switch orbitals would be computed by the Landau–Zener formula (Wittig 2005). This viewpoint has been pursued further in the later literature, especially in the context of MM models (Schütte and Wilets 1978, Nörenberg 1983, Matev and Slavov 1991) but the challenges of implementing a microscopic theory has prevented the actual calculation of macroscopic parameters such as friction coefficients.

In the present era, computational resources are available to carry out this programme using DFT and effective interactions to compute the interaction matrix elements at level crossings. Thus, we may now make theoretical predictions of the balance between inertial and

dissipative dynamics that can be used as inputs to more macroscopic models such as the ones solved with the Langevin equation. The steps to carry out this programme could follow the strategy of the dissipative diabatic dynamics (DDD) approach (Nörenberg 1983, Nörenberg 1984, Berdichevsky *et al* 1989, Matev and Slavov 1991, Mirea 2014, Mirea 2016). This would involve the construction of diabatic PES, computing the interaction matrix elements between the configurations that cross each other, and obtaining information about the time-dependence of the motion along the path. This can be achieved by adding constraints on the velocity fields in the time-dependent evolution of the configurations so that energy is conserved, see section 8.1.2. With these additional tools one can explore the probability that there will be some excitation of the nucleus along the fission path. Namely, the probability of exciting the system from the adiabatic path to a 4-qp excited state can be computed using the Landau–Zener formula. To get an actual dissipation rate, one would need to track a large number of level crossing along the diabatic path. There are many issues that need to be studied carefully at this point such as (i) non-orthogonality of the configuration basis; (ii) validation of the level density against compound nucleus level density in the first well; (iii) breaking down of the assumptions inherent in the Landau–Zener formula at low velocities; and (iv) development of reliable statistical approximations to deal with the large number of level crossings.

3.8. Collective kinetic energy

The nuclear shape evolution generally rearranges the nucleons and it is important to understand the associated collective kinetic energy. Beyond the outer turning point, while the electrostatic repulsion tends to accelerate towards the scission point, dissipative couplings damp the motion. To connect with experiment, collective kinetic energy beyond the saddle point is particularly important, because any relative motion at scission adds to the fragment kinetic energy generated by the Coulomb repulsion following scission. While in an adiabatic description all the energy difference between the saddle point (or the outer turning point for the low-energy fission) and the scission point is converted into collective kinetic energy, for strongly non-adiabatic motion, the system will irreversibly convert most of that energy into intrinsic excitations, endowing the nascent fragments with little collective motion.

For the low-energy fission, where the motion is fairly adiabatic and the dynamics of the system is governed by a CSE, the corresponding kinetic energy can be calculated on the basis of the associated inertia tensor. For a quantitative description of the collective kinetic energy it is therefore essential to understand: the relevant collective coordinates (see section 4.1); the inertia tensor (see section 4.2); the role of non-adiabatic effects in general and during the descent to scission in particular (see section 3.12); and the role of dissipation, especially near scission. In the time-dependent approaches, the kinetic energy can be obtained by computing the collective current as the local collective kinetic energy density $\propto \boldsymbol{j}^2$, where $\boldsymbol{j}$ is the current density.

While most models agree that the pre-scission kinetic energy forms only a small part of the final fragment kinetic energy, there is no general consensus about its quantitative magnitude (Bonneau *et al* 2007, Borunov *et al* 2008, Simenel and Umar 2014, Bulgac *et al* 2019b). In general the TDDFT calculations suggest that the evolution beyond the fission barrier is strongly dissipative, and this impacts the predicted kinetic energy (Bulgac *et al* 2019b).

It should be noted that TDHF models for high-energy fission are too diabatic, as the absence of pairing leads to artificial fission hindrance (Goddard *et al* 2015). The inclusion of pairing by allowing occupation number evolution solves this hindrance problem (Matev and Slavov 1991, Tanimura *et al* 2015, Scamps *et al* 2015); see also section 3.10.

The calculation of collective kinetic energy and inertia for nuclei with an odd number of protons and/or neutrons sometimes leads to diverging quantities. While a solution to this problem

is still missing, a natural strategy would be to relax the adiabatic approximation. Note that this is also mandatory when the two nascent fragments start accelerating close to the scission point. In this context, the TDDFT is arguably the most suited method, since it naturally allows the investigation of non-adiabatic effects in macroscopic transport coefficients (Tanimura *et al* 2015). The most important challenge for the TDDFT method is the inclusion of dissipation along the fission path, together with consistent fluctuations in such a way that the fluctuation–dissipation theorem is satisfied. The real challenge for this microscopic approach will be to properly describe the energy exchange between collective and intrinsic degrees of freedom (see section 3.12 for more discussion).

3.9. Approaches based on reaction theory

Nuclear fission can be naturally formulated in the language of reaction theory. Indeed, the SF process can be viewed as a decay of a Gamow resonance, while the induced fission can be expressed as a coupled-channel problem. The description of fission cross sections in induced fission, for instance, is clearly in the domain of reaction theory.

There are two general frameworks for the reaction theory of many-particle systems, namely R-matrix theory and K-matrix theory. The R-matrix framework has been extensively used in the past to construct phenomenological treatments of induced fission (Bjørnholm and Lynn 1980). But this approach is not well adapted to microscopic calculations and has never been applied at a microscopic level. In contrast, the K-matrix theory is closely allied with the configuration-interaction Hamiltonian approach that has been very successful in nuclear structure theory. The K-matrix theory has been applied to a broad range of physics subfields, but in nuclear physics only as a framework for statistical reaction phenomenology (Kawano *et al* 2015). There are severe challenges to implementing the theory microscopically. Some of these challenges are similar to those discussed in section 3.7 in the context of microscopic DDD implementations.

First, one needs to construct a basis of non-orthogonal CHFB configurations that effectively span the important intermediate states in the fission dynamics. This may be contrasted with present approaches that rely heavily on an adiabatic approximation or TDDFT implementations. Another challenge is the need for microscopic calculation of the decay width of internal configurations to continuum final states of the daughter nuclei. Tools based on the GCM should be powerful enough to estimate the needed widths (Bertsch and Younes 2019, Bertsch and Robledo 2019). It would take a large computational effort, and to date no implementations of the GCM have be validated. However, there is some experience for nuclear decays releasing an alpha particle (IdBetan and Nazarewicz 2012) as well as simple reactions involving light composite particles (Wen and Nakatsukasa 2017).

The K-matrix reaction theory might be applied as a schematic model for testing the approximations made in other approaches (Bertsch 2020). In particular, the importance of pairing in induced fission is not well understood. As mentioned in the next subsection, fission does not occur on a reasonable time scale in pure TDHF at low energies; adding pairing via TDHFB lubricates the dynamics.

3.10. Pairing as a fission lubricant

It is often said that pairing acts as a lubricant for fission. What is meant by this assertion is that if pairing is removed from the treatment, then the evolution from the ground state to scission takes place through diabatic configurations which are often disconnected. As a consequence, mean-field time evolution is sometimes unable to find the path to scission (Goddard *et al* 2015). As realised early (Moretto and Babinet 1974, Negele 1989, Nazarewicz 1993), the pairing interaction mixes those configurations and enables smooth transitions between them

(Nakatsukasa and Walet 1998). The stronger the pairing is, the easier these transitions are, and the faster fission occurs.

Pairing also plays an important role in the traditional WKB treatment of SF. The half life is proportional to the exponential of the action, which in turn is proportional to the square root of the effective collective inertia. The latter is proportional to the inverse of the square of the pairing gap, so the stronger pairing correlations the smaller action and shorter half lives. Indeed, numerous MM studies (Urin and Zaretsky 1966, Łojewski and Staszczak 1999, Staszczak *et al* 1989) demonstrated that pairing can significantly reduce the collective action; hence, affect predicted SF lifetimes. Implications of the pairing strength being a collective degree of freedom for fission are very significant, especially for the SF half-lives (Staszczak *et al* 1989, Giuliani *et al* 2014, Sadhukhan *et al* 2014, Zhao *et al* 2016, Bernard *et al* 2019).

3.11. Statistical excitation energy

Apart from possible tunnelling, the fission path traverses the PES at finite intrinsic excitation energy.[36] It can also be thought of as the energy of the quasiparticle excitations in the fissioning nucleus. Because the intrinsic energy is fairly high, and the collective evolution is fairly slow, the system has the character of a compound nucleus. Therefore the intrinsic energy is often referred to as the *statistical* energy and characterised by a local temperature. Any dynamical model of fission must therefore take into account statistical excitation energy parameterised by a local temperature. Furthermore, it is of interest to study how the fission process develops as a function of total energy, as is conveniently done in experiments inducing fission by projectiles at variable energies. However, in the microscopic frameworks, the concept of the finite temperature is plagued by a number of conceptual and technical difficulties:

Definition of temperature. In the context of the MM approaches, an effective, deformation-dependent temperature can easily be defined following the recipes given in Ignatyuk *et al* (1980) and Diebel *et al* (1981). Given the local temperature at each point of the collective space, one can construct an auxiliary PES by damping the shell correction accordingly (Randrup and Möller 2013). This maintains a micro-canonical description of the process where the total energy is constant, yet an effective PES exists and can be used for dynamics. Such an approach is more difficult in the DFT framework. First of all, many EDFs have an effective nucleon mass well below unity, adversely affecting the relationship between excitation energy and derived temperature. Secondly, the connection between the experimental excitation energy and the finite-temperature PES has not been clearly defined and, in principle, calculations of dynamics should be carried out without its help (Pei *et al* 2009, Sheikh *et al* 2009, Schunck *et al* 2015a, Zhu and Pei 2016). In any case, it is important to have a good definition of temperature to describe the disappearance of fission barriers, the increase in fluctuations, and the damping of pairing and shell effects.

Fluctuations. At finite excitation energy the fissioning system displays statistical fluctuations in addition to its inherent quantum fluctuations. Therefore a large variety of outcomes is possible and, consequently, fluctuations of observables are significant. As is obvious from the wide spreads in mass and charge yields, it is essential that the theoretical framework allows the development of large fluctuations in the final outcome. Moreover, because the possible final outcomes exhibit a very large diversity, it is not feasible to express them as fluctuations around an average. Rather, the only practical approach would provide an ensemble of outcomes whose further fate (the primary fragment de-excitations process)

[36] For clarity, the excitation energy is the difference between the total energy and the PES energy computed in CHFB constrained to the same shape parameters. The collective kinetic energy is subtracted out to obtain the intrinsic part.

can then be followed individually and specific observables can be extracted much as an ideal experiment would be analysed. This can be achieved in probabilistic treatments using Monte-Carlo simulations.

3.12. Coupling between degrees of freedom

The adiabatic approximation has often been employed to describe SF and low-energy induced fission. In these formulations, the coupling of the adiabatic collective states to the other internal degrees of freedom is a continuing challenge. Nevertheless, it is important to assess how such couplings affect decay rates and branching ratios of the fission channel to other channels. There are models available for the coupling, e.g. Brink *et al* (1983), Caldeira and Leggett (1983), but they have never been validated in a microscopic reaction-theory setting. It is worth noticing, however, that the classical Langevin equation can be derived using the model by Caldeira and Leggett (Abe *et al* 1996). This fact might be utilised to extend the Langevin approach to the quantal (tunnelling) regime. That would be an important step for the theory of low-energy nuclear dynamics.

Another problem is that the adiabatic approximation breaks down at level crossings. In that situation, a possible approach to treat dissipation is with the DDD approach (see section 3.7).

A challenge for microscopic theory is to include adiabatic dynamics together with couplings to internal degrees of freedom. Such a method should include a consistent treatment not only for intermediate states but also for the collective inertia. Current methods to compute inertial-mass tensor rely on the adiabatic approximation (Giannoni and Quentin 1980, Matsuo *et al* 2000, Hinohara *et al* 2007, Hinohara *et al* 2008, Wen and Nakatsukasa 2020). A challenging problem is to develop a microscopic theory for the large-amplitude collective motion that takes into account non-adiabatic transitions.

Ideally, the dynamic equations would provide a time-dependent statistical density matrix rather than the time-dependent wave function produced by TDHF, TDHFB, etc. An ambitious framework for such a theory has been proposed in Dietrich *et al* (2010). It would require major additions to the present coding algorithms as well as availability of high-performance computing resource to implement.

3.12.1. One- and two-body dissipation mechanisms. In the theory of heavy ion reactions, it has been long recognised that there are two distinct mechanisms that arise in a semi-classical approach to dissipation (Sierk and Nix 1980, Randrup and Swiatecki 1984). The one-body dissipation operates at the level of TDDFT. It is fast when it is present because the relevant time scale is the time it takes a nucleon to transverse the nucleus. The two-body dissipation is associated with nucleon–nucleon collisions which are largely blocked at the Fermi surface; its time scale is much longer. Quantum mechanically, it requires theoretical frameworks beyond mean-field theory, for example, the inclusion of quasiparticle excitations in the time-dependent wave functions.

In the semi-classical theory, the one-body dissipation can be encapsulated in two formulas, the wall formula for the internal dissipation in a large nucleus, and the window formula for heavy ion reactions. Both have been used very successfully for many years. However, the assumptions required for the validity of the wall formula may become questionable for low-energy fission dynamics: time scales are long and shape changes are highly correlated into low multipoles.

With the improvements in the computational capabilities for carrying out TDDFT, it should be possible to map out the region of validity of the semi-classical reductions much better. We now have credible evidence that the one-body dissipation in a quantum framework is adequate

to dissipate the collective kinetic energy (Wada *et al* 1993), but still not capable to produce a statistical equilibrium.

Fluctuations in collective variables. The presence of dissipation has two distinct but fundamentally related effects on the evolution of the collective variables. One is the average effect of the dissipative coupling which acts as a friction force resisting the evolution; this part is well described by the DFT. The other arises from the remainder of the dissipative effect which appears as a random force on the collective variables. These two forces are related by the fluctuation–dissipation theorem (Kubo 1966), often referred to as the Einstein relation.

As a consequence of the fluctuating force, the system is continually faced with a multitude of trajectory branchings, a situation that is very hard to encompass within the usual microscopic frameworks. That mean-field approaches, such as TDHF, are not suitable for describing collective fluctuations has become especially apparent after the advent of the variational approach by Balian and Vénéroni (Balian and Vénéroni 1981) who also proposed an alternative treatment of one-body fluctuations equivalent to time-dependent random phase approximation (TDRPA) (Balian and Vénéroni 1984). The practical applications of this method to fission are still limited (Scamps *et al* 2015, Williams *et al* 2018) and further developments of the formalism are required. A more radical approach would be to develop treatments that automatically endow the collective variables with fluctuations by making their evolution explicitly stochastic, as discussed in section 3.12.2.

Time-dependent generator coordinate method. A quasiparticle HFB vacuum is not expected to be a good approximation for long-time evolutions. A simple estimate leads to the conclusion that the lifetime of such state is of the order of 100–200 fm c^{-1}, whereas the time it takes from the saddle to scission might exceed several thousand of fm c^{-1}.

For the long time evolution, the mean-field state is expected to couple to the surrounding many-body states leading both to the breakdown of the mean-field picture, and to a dispersion beyond mean field in the collective space (Goeke and Reinhard 1980, Goeke *et al* 1981). This dispersion is usually described by the TDGCM (time-dependent GCM).

However, there are a number of limitations in current applications of the TDGCM to fission that all employ the GOA. For the moment, most implementations assume that the collective motion stays in the adiabatic PES. With this assumption, the manifestation of non-adiabaticity, and henceforth a proper description of the transfer of energy from collective motion to internal excitation, cannot be achieved. Extending the TDGCM approach beyond the adiabatic limit (Bernard *et al* 2011, Regnier and Lacroix 2019) to incorporate dissipation and internal excitation, will require broadening the CSE picture for the collective degrees of freedom; see, for instance, Dietrich *et al* (2010).

The internal equilibration process. Once the energy is transferred from the collective to the internal degrees of freedom, it should be understood how the energy is subsequently being redistributed so that internal statistical equilibrium is approached.

The onset of equilibration in interacting many-body systems is a long-standing problem and several theories have been proposed to treat this process (Abe *et al* 1996, Lacroix *et al* 2004, Simenel 2010). In most treatments, it is assumed that repeated in-medium Pauli-suppressed two-body collisions lead the internal degrees of freedom towards statistical equilibrium on a time scale that is relatively short compared with that of the macroscopic evolution.

One example is the extended TDHF approach (Wong and Tang 1978, Wong and Tang 1979, Lacroix *et al* 1999) or its extensions based on the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy, generically called time-dependent density matrix (Cassing and Mosel 1990, Peter *et al* 1994). These approaches have rarely been used in nuclear reactions (Tohyama and Umar 2002, Assié and Lacroix 2009) and specific technical problems seem to strongly jeopardise the

obtained results (Wen *et al* 2018). However, a promising step forward has been achieved with the purification technique, opening new perspectives (Lackner *et al* 2015, Lackner *et al* 2017).

Apart from these technical issues, this approach has the advantage that it leads naturally to the Boltzmann-like description. However, during fission, especially as the system passes through the barrier region, the excitation energy is sufficiently low to cause quantal and thermal fluctuations to coexist. This may lead to non-Markovian effects in the macroscopic evolution, which obviously would complicate the treatment. An extension of the TDGCM approach has been proposed for including thermal fluctuations (Dietrich *et al* 2010), while quantum approaches treating the thermalisation process have proven to be rather complicated. To circumvent them, approximate treatments have been suggested, including the relaxation-time approximation; see Reinhard and Suraud (2015) for recent developments.

3.12.2. Stochastic dynamics. Microscopic treatments of dissipation are discussed in section 3.7 and the previous section. Such a level of detail can be avoided by a macroscopic transport approach, treating its parameters phenomenologically. The equations here describe the evolution of just a few collective properties, typically the shape of the fissioning system, as the initial compound nucleus evolves into two separate fragments. Because the retained collective degrees of freedom are coupled dissipatively to the internal system, the macroscopic evolution has a stochastic character and the natural formal framework is the Langevin transport equation. This treatment has been very successful (Sierk 2017, Usang *et al* 2019) in calculating a variety of fission observables. A particular advantage of the Langevin dynamics is that it automatically allows the collective trajectory to undergo dynamical branchings, thereby making it possible for the system to evolve from a single shape to a large variety of final configurations.

Once the collective degrees of freedom have been identified, the Langevin equation requires three ingredients: the (multi-dimensional) PES, the associated inertia tensor, and the dissipation tensor describing the coupling to the internal system and giving rise to both the collective friction force and the diffusive behaviour of the collective evolution. It is straightforward to apply microscopic theory to determine the first two of these key quantities. For example, recent calculations of spontaneous-fission mass and charge yields (Sadhukhan *et al* 2016, Sadhukhan *et al* 2017, Matheson *et al* 2019), employed DFT to obtain the PES and the inertia tensor as a function of several collective coordinates, then performed a WKB action minimisation for the tunnelling, and a subsequent Langevin propagation until scission using a schematic dissipation tensor and random force. Such a hybrid approach can be extended to the calculation of other fission observables, such as the shapes and kinetic energies of the fragments.

The microscopic justification for the parameterised dissipation tensor remains a problem. As we have seen previously, TDDFT includes one-body dissipation mechanisms. However, dissipation cannot take place without fluctuations but it is not clear how to include the fluctuations in the microscopic treatments. Fluctuations inherent in individual configurations of HF or HFB can be addressed by the stochastic mean-field approach, which makes a statistical assumption on the origin of fluctuations, see Ayik (2008), Lacroix and Ayik (2014), Tanimura *et al* (2017) and references therein. In this approach, the noise only stems from the initial conditions. However, as it is well known in open quantum systems theory, complex initial fluctuations can lead to a stochastic dynamics with Markovian and non-Markovian noise continuously added in time during the evolution. Understanding the connection between initial fluctuation in collective space with the microscopic Langevin approach on one side, and the link with current phenomenological Langevin approaches on the other, should be addressed in the near future.

In parallel, attempts have been made to reformulate quantum theories leading to thermalisation as a stochastic process between quasiparticle states (Reinhard and Suraud 1992, Lacroix 2006) and important efforts are being made nowadays in condensed matter physics to apply

these methods (Slama *et al* 2015, Lacombe *et al* 2016). For the moment, such reformulation have been essentially made assuming jumps between Slater determinants, and equivalent formulations including superfluidity is desirable for fission. A specific problem is again that at very low excitation energy, stochastic approaches might face the difficulty of exploring rare processes.

3.12.3. Dissipation tensor. As is clear from the discussion in previous sections, dissipation plays a key role in fission dynamics. Langevin transport treatments of the collective evolution (Karpov *et al* 2001, Sierk 2017) employ the simple wall and window formulas (see section 3.12.1) in various variants, for example the chaos-weighted wall friction (Pal and Mukhopadhyay 1998). In many calculations, the dissipation tensor was phenomenologically adjusted to reproduce experimental results. In recent transport studies (Usang *et al* 2016, Usang *et al* 2017), both the dissipation tensor and the inertial-mass tensor were derived microscopically within the locally harmonic linear response approach as outlined in (Ivanyuk and Hofmann 1999), but a validation of this method still remains to be carried out.

In general, one-body dissipation is rather insensitive to the local nuclear temperature (whereas two-body dissipation is strongly energy dependent, especially at low energy where the Pauli blocking is effective). Recent studies (Sadhukhan *et al* 2016) have shown the importance of dissipation in fission, even at energies relevant to SF (Dagdeviren and Weidenmüller 1987). As a consequence, the shape evolution acquires the character of Brownian motion and many resulting observables, most notably the fragment mass distribution, are rather independent of the specific dissipation strength employed (Randrup *et al* 2011, Sierk 2017, Sadhukhan *et al* 2016).

One observable that is somewhat sensitive to the dissipation strength is the final fragment kinetic energy, a quantity that has proven to be difficult to treat reliably in models. By contrast, the time elapsed from the crossing of the fission barrier until scission is quite sensitive to the dissipation, being roughly inversely proportional to its strength. However, this quantity is difficult to measure directly, though somewhat equivalent experimental information can be obtained from quasi-fission processes (Williams *et al* 2018, Banerjee *et al* 2019).

It is an important challenge to derive the dissipation tensor from microscopic models. For this, the TDDFT method (including pairing) might be a suitable tool. In its basic form, by energy conservation and by the knowledge of the kinetic energy and excitation of the nascent fragments after scission, one can determine the total energy dissipated from the initial condition. (The excitation of the nascent fragments is initially partly given in the form of distortion energy which will gradually be converted to additional internal excitation as the fragment shapes relax to their equilibrium forms.) Two existing approaches might be useful for obtaining information on dissipation in TDDFT. The first is the density-constrained TDHF method of section 3.2.2. More systematic application of this approach to disentangle the collective energy from the excitation energy without imposing the adiabatic approximation is desirable. An alternative approach, called dissipative-dynamics TDHF, consists in making a macroscopic mapping of the collective evolution (Washiyama and Lacroix 2008, Washiyama *et al* 2009) which, however, requires a somewhat ambiguous choice of the relevant collective coordinates. This approach has not yet been applied to the fission problem, although a first step in this direction has been made (Tanimura *et al* 2015).

4. Many-body inputs

The treatment of collective nuclear dynamics in fission requires a variety of inputs that can be obtained from many-body theory.

4.1. Collective degrees of freedom

The starting point in the study of large amplitude collective dynamics is the identification of the degrees of freedom to go into the equations of motion. Although collective coordinates are not direct observables, they are treated as physical degrees of freedom; they are required for the construction of the PES as well as the associated inertia- and dissipation tensors. To achieve a satisfactory description of fission observables, such as the fragment mass distribution or the total fragment kinetic energy, it is essential to include a sufficiently rich set of collective coordinates. For example, even though the principal fission degree of freedom is the overall elongation, it is necessary to also include a shape coordinate breaking reflection symmetry to obtain realistic fragment mass yields. It was argued long ago (Nix 1969) that a reasonable description must use a minimum of five degrees of freedom, namely overall elongation, necking, reflection asymmetry, and the shapes of the two emerging fragments. It appears that an overall intensity of pairing correlations, treated as a degree of freedom, should also be added to this list (Staszczak *et al* 1989, Giuliani *et al* 2014, Sadhukhan *et al* 2014, Zhao *et al* 2016, Bernard *et al* 2019). However, the number used in actual studies is often smaller, primarily due to computational considerations.

Within the framework of MM treatments, the principal collective degrees of freedom are those characterising the nuclear shape. A variety of shape families have been employed. Probably the most widely used are the three-quadratic-surface parameterisation in Nix (1969), and the parameterisation of Brack *et al* (1972), which have three parameters. A detailed discussion of the advantage of one particular parameterisation over another can be found in Möller *et al* (2009). However, even five shape degrees of freedom may not always be sufficient. For example, triaxial shape deformations are often important in the region of the first saddle.

Self-consistent treatments based on nuclear EDFs have used multipole moments of the matter distribution as constraints to play the role of collective coordinates (Krappe and Pomorski 2012, Younes *et al* 2019). The primary collective coordinates employed in such studies are the quadrupole moments Q_{20} and Q_{22} used to control the overall distortion and triaxiality of the system, respectively, the octupole moment Q_{30}, used to control its reflection asymmetry, and the neck parameter or the hexadecapole moment Q_{40}. An interesting possibility is to generalise the use of a set of multipole moments as the constraining operators by using the density distribution itself, see section 3.2.2 for further discussion.

It is important to recognise the principal difference between the use of the nuclear shape as a (multi-dimensional) collective variable, as is done in the macroscopic–microscopic approaches, and the use of a set of density moments, as is being done in the microscopic treatments. Whereas the former approach calculates the properties of the system having the specified shape, the latter automatically performs energy minimisation so the system being treated is the one having the lowest energy subject to the specified moment constraints. Consequently its shape (or more generally: its matter distribution) is not under complete control. As discussed in section 3.2.1, the self-consistent density distribution may exhibit discontinuities as the moments are varied smoothly as a small change in the constraints might cause the new minimal state to have a quite different spatial appearance. This problem is particularly severe near the scission point, where there might be a major reorganisation of orbital fillings. A recent detailed study of this problem (Dubray and Regnier 2012) developed diagnostic tools for identifying its presence and demonstrated how additional constraints could help. In any case, no set of collective coordinates were found that could eliminate the problem entirely. It is therefore clear that at least three collective constraints are needed to mitigate such discontinuities.

Fluctuations of the pairing field have also been used as collective coordinates (Staszczak *et al* 1989), see section 3.10. Here, a constraint on the dispersion in particle number

$\langle N^2\rangle - \langle N\rangle^2$ is imposed to control the strength of the pairing field (Vaquero *et al* 2011, Vaquero *et al* 2013). Studies of fission dynamics have shown that the coupling between shape and pairing degrees of freedom has in fact a significant effect on the collective inertia and, therefore, on the dynamical paths in the collective space. In particular, it may have a pronounced influence on SF half-lives (Sadhukhan *et al* 2014, Zhao *et al* 2016, Bernard *et al* 2019). Pairing coordinates may also be important for the odd–even staggering in the fission yields (Mirea 2014, Rodriguez-Guzmán and Robledo 2017). Induced fission is traditionally treated in a finite-temperature framework, where pairing is quickly quenched by the statistical fluctuations. Here, again, the dynamical treatment of pairing could substantially change the picture.

Generally, the introduction of additional collective coordinates increases the required numerical effort significantly. Nevertheless, for more refined descriptions, there is a need for a few additional collective variables that are not shape-related. One is the projection of total angular momentum on the fission axis, usually denoted by K (Nadtochy *et al* 2012, Bertsch *et al* 2018), which affects the angular distribution of the fission fragments. In a recent study, the configuration space was constructed in the HF approximation using the K-partition numbers as additional constraints (Bertsch *et al* 2018).

Another additional collective degree of freedom is related to the isospin. Except for TDHF, TDHFB, and DFT-Langevin, fission treatments have usually assumed that the fragments retain the same proton-to-neutron ratio as that of the mother nucleus. While some progress has recently been made in incorporating this degree of freedom into the MM treatments (Möller *et al* 2014, Möller and Ichikawa 2015, Möller and Schmitt 2017), further developments are still needed.

A near-term challenge will be to take advantage of newly available extensive computing resources and expand the space of collective coordinates, with the aim of obtaining a more realistic description of the evolution of the fissioning nucleus into fragments, especially in the region where nascent fragments appear near and beyond scission.

4.2. Collective inertia

The ATDHFB (adiabatic time-dependent HFB) and GCM + GOA formalisms are often applied to derive collective inertias for the CSE. In the ATDHFB this requires the inversion of the full linear response matrix. From a computational point of view, this is a daunting task that has been often alleviated by imposing various approximations (Schunck and Robledo 2016). Typically, fission calculations rely on the ATDHFB inertias within the so-called non-perturbative cranking approximation, where the non-diagonal terms of the linear response matrix are neglected and the derivatives of the generalised density matrix with respect to the collective variables are computed numerically (Baran *et al* 2011). Very recently, both the exact and non-perturbative cranking GCM + GOA inertias have been computed for the first time (Giuliani and Robledo 2018), showing that the non-perturbative cranking ATDHFB inertias can be reproduced even without the inclusion of collective momentum variables.

In the TDGCM framework, the expression for the collective kinetic energy can be obtained using either the GCM or the ATDHFB formalism. While the latter approach leads to the physical inertia in the case of translational motion (Ring and Schuck 1980), the GCM approach may be incorrect if the conjugate collective variables are not included as collective degrees of freedom. This requires doubling the dimensionality of the collective space and in practice this is rarely if ever done (Goeke and Reinhard 1980). To obtain a more realistic inertia, the ATDHFB expression is sometimes used in the GCM approaches. The possibility of using fully consistent GCM with pairs of collective variables would be desirable in the future.

Given the current status, several aspects should be addressed in order to reduce the source of uncertainties in the estimation of collective inertias. Among the most impelling ones is the calculation of the exact ATDHFB inertias. This is desirable because, according to the instanton formulation (see Skalski (2008) and section 3.6), it is the ATDHFB that provides a compatible framework to tackle the problem of nuclear dynamics under the barrier. The full linear response matrix has been inverted in Lechaftois *et al* (2015) under some approximations but this method has not yet been extended to fission studies. Alternatively, one could try an approach along the lines of the finite amplitude method (Hinohara 2015), where rather than inverting the linear response matrix itself one computes its action on the time derivative of the density matrix entering in the expression of the collective inertias. Such an approach has already been proposed and tried long time ago (Dobaczewski and Skalski 1981), and, as advocated in Dobaczewski (2019), the time is ripe to start implementing it routinely in all ATDHFB calculations. Regardless of the practical implementation, the estimation of the exact ATDHFB inertias is a crucial step to understand the validity of the non-perturbative cranking approximations, which will reduce the uncertainties related to the collective inertias and bring a sounder estimation of collective kinetic energies and in the general adiabatic description of the fission process.

When it comes to non-adiabatic formulations, collective inertia can be derived within the DDD formalism (Mirea 2019). For low collective velocities, the DDD inertia reduce to the cranking expressions.

4.3. Collective dissipation

In most treatments of the fission dynamics based on microscopic theory, it has been assumed that the collective degrees of freedom are well decoupled from the intrinsic degrees of freedom, usually referred to as the adiabatic assumption. Unfortunately, the nuclear A-body wave function of the nucleus cannot, in general, be expressed in terms of slow and fast components. Indeed, the typical time scale of nuclear collective modes is only slightly greater than the single-particle time scale (Nazarewicz 2001). In the context of fission, the adiabatic approximation is questionable as the collective motion is highly dissipative (Blocki *et al* 1978, Bulgac *et al* 2019b), see section 3.5.

There is therefore an urgent need for addressing the collective dissipation within a microscopic framework. While this presents a significant computational undertaking, the most immediate task consists in deriving the appropriate expressions for the dissipation in the particular microscopic model employed, a problem that is still quite unsettled (Barrett *et al* 1978). Another challenge is to identify high-quality fission data that will constraint the dissipation tensor.

4.4. Level densities

The nuclear level density is a key ingredient of the Hauser–Feschbach statistical theory of nuclear reactions. Modelling many aspects of fission reactions rely on this type of statistical reaction theory: a first example is nucleon-induced fission, where the capture of the projectile by the target and the fission of the resulting compound nucleus are treated as a two-step process. Another example is the prompt de-excitation of the nascent fission fragments, which can be treated as compound nuclei undergoing statistical decays. Especially for applications in nuclear astrophysics, such as the calculation of fission transmission coefficients and fission yields, reliable predictions of nuclear level densities over a broad range of excitations for a large region of nuclei are desired.

Three main classes of nuclear level density models exist: analytical models (such as the back-shifted Fermi gas), configuration-interaction methods, and combinatorial model. Due to

their simplicity, analytical models are often used in reaction codes, but they do not account for specific nuclear structure effects to a satisfactory degree. While in principle very powerful, configuration-interaction shell-model methods have so far been applied only to a limited number of light and medium-mass nuclei because of their computational complexity. In contrast, the shell-model Monte Carlo (SMMC) approach is capable of calculating level densities of heavy nuclei and was applied to nuclei as heavy as the lanthanides (Alhassid *et al* 2008). SMMC level densities have the advantage that they include contributions from both intrinsic and collective excitations. However, application of SMMC across the nuclear chart will require large computational resources.

Combinatorial models do not suffer from this hurdle and have been applied on the scale of the nuclear chart. These are usually based on the microscopic single-particle levels (provided by DFT calculations, microscopic–macroscopic approaches, or analytical optical potentials) from which the many-quasiparticle excited states are obtained after pairing has been included. The level density obtained by such combinatorial counting must be augmented by the effect of excited states that are mostly collective in nature. Most important is the appearance of rotational bands for deformed nuclei which may increase the level density by more than an order of magnitude even at moderate excitation energies. Even though this effect is very important, most treatments have long included it only by means of an empirical formula based on the moment of inertia of the nucleus (Bjørnholm *et al* 1973). However, more recent approaches have considered each individual many-quasiparticle excited state to be a rotational bandhead (Uhrenholt *et al* 2013), thus avoiding the introduction of adjustable parameters. Collective vibrations have also been included (Hilaire *et al* 2012, Uhrenholt *et al* 2013), but these are most often neglected as they have been found to have only a small impact at low excitations compared to the rotational enhancement.

An additional aspect of the modelling of these collective enhancements is their dependence on the nuclear shape. For example, photofission rates are sensitive to the ratio of level densities at the ground state and at the fission saddle point. Many transport models use the level density (as a function of the collective coordinates) to relate the local excitation energy to a local temperature. Furthermore, recent transport treatments of fission have employed shape-dependent level densities to guide the nuclear shape evolution (Ward *et al* 2017), an approach that automatically takes account of the gradual decrease of pairing and shell effects at increasing excitation. The effect of this energy dependence is often emulated by using a phenomenological damping function for the level density. Finally, shape-dependent microscopic level densities are also important for the division of the internal excitation energy between the pre-fragments at scission (Albertsson *et al* 2020).

Statistical quantities are important in many aspects of fission, and microscopic theory is needed to go beyond the current empirical modelling of their dependence on shape and other variables. Particularly challenging is the problem of calculating shape-dependent level densities with a proper description of the gradual erosion of the shell effects with increasing energy.

5. Initial conditions

Nuclear fission can proceed from a variety of initial states; see section 2.1. In addition to SF, the process can be induced by a variety of nuclear reactions that lead to the initial state of the fissioning (mother) nucleus. Figure 3 displays some characteristic time intervals for the preparation of the initial state. The reaction types are roughly ordered by the amount of energy they may bring into the compound system, with the most energetic reactions (‘fast probes’) on

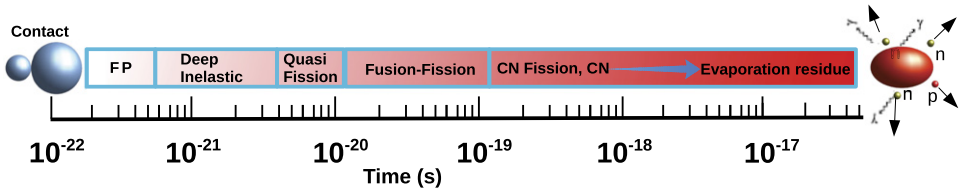

Figure 3. Time scales for various reactions that may induce fission in large nuclei. FP means fast probes and CN stands for compound nucleus.

the left. On the right, labelled 'CN fission', are the more gentle probes such as neutron capture that proceed through the compound nucleus.

5.1. Neutron-induced fission

Due to its importance in applications, low-energy neutron-induced fission is probably the best experimentally studied and phenomenologically parameterised fission process. Proceeding through narrow neutron resonances, it creates the nucleus in a long-lived excited state that has enough time to thermalise the absorbed energy, thus forming a compound nucleus.

The incident neutron creates a compound nucleus at an excitation energy that can range from somewhat below the barrier to energies above the barrier. As the neutron energy is raised, the resulting excitation may make it possible for the nucleus to evaporate one or more neutrons before fissioning (referred to as a multi-chance fission). At still higher energies, non-equilibrium emission grows important and a thermalised compound nucleus is established only after the loss of one (or possibly more) nucleons.

The representation of the initial compound state in terms of elementary excitations is impractical because the level density is prohibitively high. Thus a direct description in terms of QRPA modes, GCM excited states, etc, would not be feasible and it may be preferable to adopt an approach based on statistical quantum mechanics. However, for the neutron-induced fission close to the neutron drip line, where level densities at the neutron separation energies are small, the process could still be dominated by the direct component rather than the compound one.

Besides the energy, all the quantum numbers of the formed compound nucleus may affect the subsequent fission process, especially when the energy is close to the barrier height. This level of detail is retained in the *R*-matrix theory, discussed in section 3.9.

5.2. Fission induced by fast probes

Fission can be induced by fast probes such as photons (photofission), charged particles, and high-energy neutrons. Surrogate reactions, such as fission following multi-nucleon transfer reactions, are also included here. In these processes, the nucleus is created in an excited state above or below the fission barrier. This state may exhibit specific well-defined structures, such as the giant dipole resonance, which have substantial widths.

Present theoretical descriptions of fission induced by fast probes most often assume the creation of a compound nucleus at a given thermal excitation energy (cf the process of neutron-induced fission discussed in section 5.1). However, for fast probes such an assumption might be ill-founded because the nuclear system may not have sufficient time to thermalise before undergoing fission. Therefore, a non-thermal description of fission at high excitation energies is very much desired (Dobaczewski 2019).

This becomes increasingly important at higher energies where pre-equilibrium processes play an increasingly significant role and may lead to the emission of one or more nucleons

before equilibrium is reached. Moreover, as the excitation energy of the compound nucleus is increased, neutron evaporation competes ever more favourably with fission and, as a result, multi-chance fission is likely to happen.

5.3. Formation by electromagnetic and weak-interaction fields

5.3.1. Photofission. In photofission, a nucleus decays through the fission channel after absorbing a high-energy photon—a γ-ray. The characteristics of the excited state resulting from photo-absorption—the initial state for the fission process—determines the evolution of the system, for instance, by determining whether enough excitation energy is available to surmount the fission barrier. Thus, the knowledge of excited states above both the ground state (for fissile nuclei) and shape isomers, as well as multipole transition probabilities between these states, is in principle needed to model photo-absorption as a function of the photon energy. If the photon is absorbed through the dipole operator on an even–even nucleus, the angular distribution of the fission fragments gives information about the mixing of the K quantum number in the fission process. In general and outside of the giant dipole absorption peak, theories such as the QRPA are needed to sort out the multipoles.

5.3.2. Coulomb excitation. Another electromagnetic excitation method to study fission of heavy nuclei in a relativistic accelerator beam is Coulomb excitation. Here, the process can be treated as excitation by virtual E1 photons, so the considerations in the previous paragraph apply. While the energy transferred is not precisely known, the theory for its distribution is well established.

5.3.3. β decay and electron capture. Fission of nuclei far from stability can sometimes be studied when the nuclide is formed by β decay of a progenitor nuclide. In terms of the excitation energy, β-delayed fission is intermediate between SF and Coulomb-excitation induced fission. Importantly, this process makes it possible to study low-energy fission in proton-rich heavy nuclei that are not accessible by other techniques (Andreyev *et al* 2013). As in Coulomb excitation, the excitation energy given to the nucleus is not known precisely. Thus the theory of β-decay strength function is required to model the whole process. In this regard, the QRPA (in its charge-exchange formulation) is very valuable.

The process of β-delayed fission also plays an important role in nucleosynthesis, because it helps to terminate the rapid-neutron-capture process. Fission may occur from the compound nuclei created by neutron capture or from the β-decay daughters of those nuclei (Mumpower *et al* 2018). The latter can happen whenever the β decay populates a daughter state with an excitation energy above (or near) the height of the fission barrier. Since it is important to know the spin and the parity of the initial state before fission, the description of β-delayed fission requires a microscopic model of the charge-exchange process to provide β-strength distributions; for the recent QRPA work see Mustonen *et al* (2014), Mustonen and Engel (2016), Shafer *et al* (2016). The QRPA applications used to describe β-decay are often limited to allowed transitions. Thus it would be necessary to extend many current QRPA codes to enable computation of all possible final states in daughter nuclei.

Because β-delayed fission often involves odd–odd nuclei, one should employ a formalism that can be extended to such systems without introducing any additional approximation. Therefore, both the underlying HFB solver as well as the QRPA implementation should break time-reversal symmetry, that is, extend beyond the equal filling approximation. This last point is essential to differentiate between low- and high-spin states in odd–odd nuclei, and thus distinguish between decays from potential isomeric states and the ground state. Once the fissioning daughter state has been determined, one should be able to calculate the corresponding PES for the particular energy, spin, and parity.

5.4. Heavy-ion reactions

In the search for superheavy nuclei, the experiment uses a heavy-ion reaction to fuse together two large nuclei, hoping that the combined system equilibrates and then decays as a compound nucleus. Cross sections can be estimated for this reaction mechanism, but a crucial ingredient is the probability to form a compound nucleus. The reaction is called fusion–fission in that case; if there is no equilibration it is called quasifission. The understanding of this distinction requires a combination of statistical and truly dynamical approaches which are not necessarily confined to a collective subspace. Quasifission leads to the formation of products that may have similar properties to fission products, but are produced without the formation of compound nucleus. Fusion–fission occurs after the formation of a composite system which fissions due to its excitation, resulting in a fragment distribution that is peaked at equal mass breakup of the composite system. This difference in fragment distributions indicates that quasifission is the faster process and corresponds to a system that is not yet fully equilibrated. As a dynamical process, quasifission is amenable to a description using the TDHF approach (Simenel and Umar 2018). A number of TDHF studies of heavy-ion reactions have been reported in recent years (Wakhle *et al* 2014, Oberacker *et al* 2014, Umar *et al* 2016, Godbey *et al* 2019, Sekizawa 2019, Godbey and Umar 2020). In general, the TDHF results agree well with the experimental quasifission yields, and shed light on some of the underlying reaction dynamics in relation to target/projectile combinations.

Quasi-fission and fusion–fission could be used to map out the non-adiabatic collective landscape between the fusion entrance channel and the fission exit channel. The calculated time scales indicate that while fast quasifission events dominate, much slower events resulting in a fracture with equal mass fragments have also been observed.

One of the open experimental questions is how to distinguish quasifission from fusion–fission. This is important for calculation of the evaporation residue formation probability in superheavy element searches. A collaborative effort between theory and experiment is needed to find ways to address these issues. One may try to 'calibrate' the experimental quasifission yields with the help of theoretical simulations thus allowing the extraction of the fusion–fission yield. Study of angular distributions (now routinely measured with large angular acceptance detectors (Banerjee *et al* 2019)) may be one of the ways to approach this task.

Theoretical studies of quasifission have taught us that the dynamics may be dominated by shell effects (Simenel and Umar 2018, Sekizawa 2019). Despite the apparent strong differences between fission and quasifission, it is interesting to note that similar shell effects are found in both phenomena (Scamps and Simenel 2018, Scamps and Simenel 2019, Godbey *et al* 2019). Quasifission can then potentially be used as an alternative mechanisms to probe fission mode properties. For instance, this could provide a much cheaper way than fusion–fission to test the influence of the ^{208}Pb shell effects in super-asymmetric SHE fission. Note that this approach would only provide information on the properties of fission modes (mass asymmetry, TKE, excitation energy), but not directly on their competition. Indeed, the latter is likely to be determined near the saddle point, a region of the PES which is not necessarily explored by the quasifission paths.

6. Forces for fission dynamics

The collective fission dynamics can be understood as a balancing of three different types of forces: the driving forces arising from the generally multi-dimensional potential energy of deformation of the fissioning system, the inertial forces caused by the macroscopic rear-

rangement of the nucleons associated with the change of the collective coordinates, and the dissipative forces arising from the coupling of the considered collective coordinates to the remainder of the nuclear system. In a microscopic approach these fission-driving forces are derived from the effective inter-nucleon interactions, which are optimised to selected data.

6.1. Energy density functional

In a microscopic approach to fission, the effective inter-nucleon interaction or EDF is the only ingredient of the theory that includes adjustable parameters. Therefore, the choice of a functional ultimately determines the quality of the microscopic description of phenomena related to fission, and the level of quantitative agreement with data.

Several types of EDF have been proposed over the years, many of which have also been applied to fission. These functionals can be non-relativistic or relativistic (or covariant), and this choice leads to different equations of motion for nucleons; they can be functionals of local or non-local densities; they can be strictly defined as the expectation value of a corresponding generating many-body operator or not; and finally the couplings (parameters) can be constants or include a medium (density) dependence.

The two most widely used non-relativistic EDFs (Bender *et al* 2003, Schunck 2019) are the finite-range Gogny EDF, which is constructed including the HFB expectation value of a density-dependent interaction, and the Skyrme EDF, which includes momentum- and density-dependent zero-range terms in the interaction. Other types of local non-relativistic EDFs that were recently developed and applied to detailed studies of fission processes are the Barcelona–Catania–Paris–Madrid (Baldo *et al* 2013), SEI (Behera *et al* 2016), and SeaLL (Bulgac *et al* 2018) EDFs. Similarly, there are several varieties of relativistic EDFs in use (Schunck 2019, Agbemava *et al* 2017, Agbemava *et al* 2019), either with finite-range (meson-exchange) or contact interaction potentials, with non-linearities in the meson and/or nucleon fields, or including density-dependent couplings. Two relativistic point-coupling (contact) functionals, in particular, have successfully been applied to studies of fission dynamics: PC-PK1 (Zhao *et al* 2010) and DD-PC1 (Nikšić *et al* 2008).

One important challenge is to increase the predictive power of novel nuclear EDFs compared to traditional functionals such as Gogny or Skyrme, which apparently cannot be improved further (Kortelainen *et al* 2014). For instance, the density-matrix expansion (Carlsson and Dobaczewski 2010, Gebremariam *et al* 2010, Gebremariam *et al* 2011, Stoitsov *et al* 2010) can be used to construct nuclear EDFs that are guided by first principles (Dyhdalo *et al* 2017, Navarro Pérez *et al* 2018, Zhang *et al* 2018). Extensions of time-tested EDFs have been subject to recent studies. For example, higher-order gradient terms have been added to the Skyrme EDF (Carlsson *et al* 2008, Davesne *et al* 2013, Becker *et al* 2017). The Gogny family of functionals have been extended to include additional density-dependence and tensor interactions (Chappert *et al* 2015, Pillet and Hilaire 2017, Bernard *et al* 2020). One hopes that such extensions would augment the parameter space to be optimised for a better description of fission properties.

Over the past decade it has been realised that exact projection techniques (see section 3.4.2) and exact GCM are ill-defined for EDFs that are not strictly constructed from an effective Fock-space Hamiltonian (Anguiano *et al* 2001, Dobaczewski *et al* 2007, Lacroix *et al* 2009, Bender *et al* 2009, Duguet *et al* 2009, Robledo 2010b). The basic dilemma that one faces in this context is that a suitable form of an effective Hamiltonian that reaches the descriptive power of conventional EDFs has not yet been identified. As a first step in this exploration, a scheme for a systematic construction of flexible two-body interactions by combining finite-range Gaussians and gradients, has been proposed (Dobaczewski *et al* 2012, Bennaceur *et al* 2017). Limiting

oneself to a two-body interaction, however, will inevitably lead to an unrealistically small effective mass (Davesne *et al* 2018), such that one always has to add three-body, and perhaps even higher, interactions. The computationally simplest form of such terms is provided by contact three-body forces with gradients (Sadoudi *et al* 2013). It turns out, however, that when added to two-body interactions of various forms, they do not offer sufficient flexibility, which makes this quest even more challenging.

Many advanced methods for beyond-DFT modelling of fission dynamics often include explicit correlation energies that were implicit in the effective interaction obtained from the EDF optimisation. This inconsistency may degrade the descriptive and predictive power of the model and should be avoided. A better strategy would be to optimise the EDF parameters using data sensitive to large deformations. This issue is most obvious in the case of corrections for quantal zero-point motion related to symmetry breaking and shape fluctuations, such as those for the centre-of-mass, rotational, and shape-vibrational motion. For instance, the inertia that determines the former is the mass number A, which becomes ambiguous whenever one considers the separation of a single nucleus into fragments (Goeke *et al* 1983, Skalski 2006). The rotational correction increases with deformation and therefore lowers fission barriers, etc. To further complicate matters, one form of quantal correction is transformed into other forms when changing deformation (Goeke *et al* 1983, Skalski 2006), such that from this point of view many quantal corrections have to be treated simultaneously. The same considerations also apply to exact projections and full GCM.

Static and dynamic pairing correlations play a crucial role for the calculation of deformation energy surfaces, the dynamic fission path, and collective inertia. This means that the pairing part of the effective interaction or EDF might have to be tailored in such a way to reproduce both ground-state properties and selected features that determine fission data, see section 6.2.

6.2. Optimisation strategies

Once the form and the framework for which the parameters of an EDF are to be adjusted are decided, the next question concerns the selection of fit observables. Most of the fission observables (lifetimes, fission fragment distributions, ...) are computationally expensive and cannot be systematically considered during the optimisation. Therefore, one has to identify properties that encapsulate the essence of the relevant physics probed by fission and, at the same time, can be computed in a reasonable time.

First of all, the EDF has to be capable of describing the structure of the initial state of the fissioning nucleus and the final state of the fragments. At low excitation energy, the requirements for this are the same as for standard nuclear structure applications. One of the most important constraints on the EDF specifically relevant for fission studies is its ability to describe states at very large deformation. Two different types of properties control the general features of fission dynamics: on the one hand the surface and surface-symmetry energy coefficients that determine the average resistance of the nucleus against deformation (Nikolov *et al* 2011, Jodon *et al* 2016), and on the other hand the evolution of shell structure that generates the minima and maxima associated with the multi-humped structure of the deformation energy landscape (Brack *et al* 1972).

There is some direct information about the excitation energy of highly-deformed states that is available and that can be used to inform the parameter fit. On the one hand, there are barrier heights data (Capote *et al* 2009, Smirenkin 1993), which have to be interpreted with some caution as in one way or the other the available values were obtained via intermediate models (Capote *et al* 2009). On the other hand, there are also measured excitation energies of some fission isomers (Singh *et al* 2002). For a very limited number of fission isomers there is also

information about their quadrupole deformation from E2 transition moments (Metag *et al* 1980, Thirolf and Habs 2002), and some information about their shell structure can be obtained from the quantum numbers of bandheads. Additional data on such states would clearly be of great help for fine-tuning the nuclear EDF.

To date, the EDFs most commonly used in fission studies have been adjusted to fission isomer excitation energies (Kortelainen *et al* 2012) or fission barriers (Bartel *et al* 1982, Berger *et al* 1991, Goriely *et al* 2007), with the exception of the relativistic functionals PC-PK1 (Zhao *et al* 2010) and DD-PC1 (Nikšić *et al* 2008) that combine information on deformed heavy nuclei and the nuclear matter equation of state. Some authors suggest paying more attention to the nucleus–nucleus interaction between pre-fragments near scission (Adamian *et al* 2016).

A technical issue that needs to be addressed is that many parameterisations of the nuclear EDF exhibit so-called finite-size instabilities, meaning that homogeneous infinite nuclear matter is unstable against a transition to an inhomogeneous phase that is either polarised in spin or isospin or both, see Pastore *et al* (2015) for a review. Finite-size instabilities can be triggered by gradient terms in the EDF, but also by finite-range terms in non-local EDFs (Martini *et al* 2019, Gonzalez-Boquera *et al* 2020). Many parameterisations of the Skyrme EDF exhibit such instability in one or the other spin channel, which becomes an issue when working with time-reversal breaking configurations or when calculating certain RPA modes. Such instabilities are also sometimes found in isovector channels of some Skyrme and Gogny parameterisations. All of these instabilities can be efficiently and unambiguously detected with linear-response calculations of infinite nuclear matter. Such test can be easily incorporated into fit protocols, as already done for the UNEDF2 (Kortelainen *et al* 2014) and SLy5sX (Jodon *et al* 2016) Skyrme parameterisations.

Irrespective of the choices that will be ultimately made for the form of the EDF and the protocol for the adjustment of parameters, it is clearly desirable to have just one or a few standard EDFs for fission studies that are used by as many groups as possible in order to eliminate possible dependencies upon the parameterisation when comparing results obtained with different approaches to treat the many-body problem. For TDDFT treatments, it is also important that EDFs are fitted without the centre-of-mass corrections (Goeke *et al* 1983, Skalski 2006, Kim *et al* 1997, Simenel 2012, Kortelainen *et al* 2012).

6.3. Uncertainty quantification

As discussed in the previous section, nuclear density functionals have to be calibrated to experimental data. This empirical wisdom is built into the quality measure $\chi^2(\boldsymbol{p})$ which is a scalar function of the N_p model parameters $\boldsymbol{p}$. The common use of χ^2 is to deduce the optimal parameterisation $\boldsymbol{p}_0$ by minimising χ^2.

Systematic uncertainties can be revealed by comparing predictions of different models; for fission applications, see Kortelainen *et al* (2012), Agbemava *et al* (2017). In the context of statistical uncertainties related to model parameters, much information can be unravelled by employing χ^2 in connection with the tools of statistical analysis (Dobaczewski *et al* 2014, McDonnell *et al* 2015, Schunck *et al* 2015c, Schunck *et al* 2015b, Nikšić *et al* 2015, Reinhard 2018).

Computing the probability distribution of the parameters $\boldsymbol{p}$ rather than a single point gives immediately access to two important new pieces of information, the uncertainty of a predicted observable, and the correlation between two observables. Uncertainties are important to control the quality of a prediction. This is mandatory when using the results in further calculations as done, e.g., in nuclear astrophysics, and it is an extremely useful indicator for model development because it reveals deficiencies of parameterisations. Correlations add another world of

information. They allow a sensitivity analysis to check the impact of a certain model parameter on an observable (Kortelainen *et al* 2010, Kortelainen *et al* 2012) and they indicate the information content of a new observable as compared to previous ones (Reinhard and Nazarewicz 2010, McDonnell *et al* 2015). In the context of the present report, it is particularly interesting to apply correlation analysis for the very different observables discussed here, e.g., relating fusion cross sections and fission properties.

There is still more potential in statistical analysis of DFT. So far, the evaluation of uncertainties and correlations has mostly been based on a Taylor expansion of the χ^2 and of observables around the optimal parameterisation $\boldsymbol{p}_0$. This runs easily beyond validity, particularly for fission properties (Higdon *et al* 2015). Thus one needs to evaluate the integrals $\int \mathrm{d}^{N_p} p \ldots$ in detail which grows quickly infeasible. Here one can take advantage of modern techniques of supervised learning. Employing the posterior probability distribution computed with emulators, one can propagate theoretical statistical uncertainties in predictions of various computed quantities, including binding energies and PESs (McDonnell *et al* 2015, Neufcourt *et al* 2018, Neufcourt *et al* 2020, Lasseri *et al* 2020). One can teach the emulators to improve the predictions of selected observables in a given region of the nuclear chart by one order of magnitude at practically no extra cost. This is particularly desirable if the output of nuclear DFT calculations is used as input in other chains of calculations as, e.g., in nuclear astrophysics simulations.

To estimate uncertainties, both systematic and statistical, uniform model mixing (Erler *et al* 2012a, Agbemava *et al* 2017) can already provide a very valuable information. More advanced techniques involve Bayesian model averaging (Neufcourt *et al* 2019, Neufcourt *et al* 2020), which allows to maximise the 'collective wisdom' of relevant models by providing the best prediction rooted in the most current experimental information. This will be an important part of future collaborative projects in fission theory.

7. Fission fragments

In the last stage of the fission process, the nucleus descends towards scission where it divides into nascent fragments, which then de-excite, see figure 1. The following sections are devoted to fission fragments and the related fission observables.

7.1. Scission

The scission event is arguably one of the least understood processes in fission, although some experimental information on scission configurations have just became available (Ramos *et al* 2020). In a mean-field picture it marks the transition from the final state of the elongated fissioning nucleus to the initial state of the two separated nascent fission fragments. As discussed later in section 7.5, there are good reasons to think that the nascent fragments are entangled at, or immediately after, scission but it is not clear whether this entanglement persists to the stage of the fission fragments or quantum decoherence takes place. Furthermore, the characteristics of these fragments such as their charge, mass, energy, angular momentum, parity, level density, etc, are crucial ingredients in determining the properties of the neutron and γ spectra, as well as the β-decay chains, see section 7.7.

Before microscopic time-dependent descriptions of fission dynamics became available, the scission event was most often treated with *ad hoc* assumptions, ignoring any role for dynamics. At one extreme, scission is assumed to transform the system into a statistical ensemble of two nuclei having their surfaces separated. In the framework of DFT theory, various criteria were introduced to define scission based on the HFB solution for the fissioning nucleus. The simplest ones define a threshold value for the density between the two pre-fragments or

the expectation value of the neck moment. The main problem with such schemes, however, is that both the intrinsic energy of each pre-fragment and their relative interaction energy are extremely poorly described: before the separation of the pre-fragments, both the nuclear and Coulomb interaction energies are vastly overestimated because of the large overlap between the pre-fragments; when the primary fragments are well separated, the minimisation principle underpinning the HFB equation leads to the two fragments in their ground state. Such dramatic simplifications can be mitigated by performing unitary transformations on the total wave function of the fissioning system which, while leaving the whole system invariant, can be designed to minimise the interaction (or equivalently, maximise the localisation) of the pre-fragments (Younes and Gogny 2011). In spite of the development of such techniques, it is clear that explicitly non-adiabatic, time-dependent methods provide a much better handle on scission—at least when it comes to defining the initial conditions of the nascent fragments.

7.2. Fission fragment yields

Three main methods are used to determine the yields of different fission fragments. Scission-point models assume a statistical distribution of probability among a set of scission configurations of the nucleus (Fong 1953, Wilkins *et al* 1976), see Lemaître *et al* (2019) and Paşca *et al* (2019) for recent realisations. These models require the definition of an ensemble of scission configurations that can either be determined by constrained mean-field calculations or from an analytical parameterisation of the shapes of the di-nuclear system. Each of these nuclear configurations is then populated according to a Boltzmann distribution, with the temperature defined in accordance with the initial energy of the system. Since it is computationally effective, this method is used in systematic studies or to investigate the evolution of yields with the excitation energy of the compound nucleus. However, the choice of the ensemble of scission configurations remains arbitrary and may influence the resulting yields. Moreover, an explicit use of temperature for a non-adiabatic and time-dependent process is not really well justified.

To some degree, also the total fragment kinetic energy may be estimated. In particular, some models have sought to predict those quantities exclusively on the basis of the scission configurations (Lemaître *et al* 2015), but their predictive power has been limited due to the importance of the collective path taken prior to scission. Indeed, experience with a diffusive transport model (Randrup *et al* 2011) has shown that not only the scission hypersurface but the global topography of the PES may have a qualitative influence on the outcome.

To avoid the assumption of statistical equilibrium at scission, one possibility is to describe the evolution of the compound nucleus from some initial state at lower deformation up to the configurations close to scission. In this approach, one defines an equation of motion for a few collective coordinates associated with a parameterised shape of the nuclear surface. Assuming that these collective degrees of freedom interact with a thermal bath of intrinsic excitations, leads to the Langevin equations in the deformation space; see section 3.5.

These transport equations have been solved in multi-dimensional spaces both in MM and hybrid-DFT frameworks either directly (Miyamoto *et al* 2019, Sierk 2017, Ishizuka *et al* 2017, Usang *et al* 2019, Sadhukhan *et al* 2016, Sadhukhan *et al* 2017, Matheson *et al* 2019) or in the strongly damped (Smoluchowski) limit (Randrup and Möller 2011, Randrup *et al* 2011, Ward *et al* 2017). The result is the probability of populating different nuclear configurations close to scission and it is then straightforward to determine the resulting mass asymmetry.

Most often these treatments have concentrated on the mass number, assuming that the proton-to-neutron ratio remains constant, but recent progress has been made (Möller *et al* 2014, Möller and Ichikawa 2015, Möller and Schmitt 2017, Sadhukhan *et al* 2016, Sadhukhan *et al* 2017, Matheson *et al* 2019) towards including also the isospin degree of freedom, thus making

it possible to determine both the mass and the charge yields. The transport framework takes into account the dissipative effects of the collective dynamics and may even account for the emission of neutrons in the course of the evolution (Eslamizadeh and Raanaei 2018). One general limitation is that the Langevin treatment is restricted to the classically allowed region of the collective space, so it cannot treat tunnelling.

As mentioned in section 3.4.1, an alternative approach to computing fission fragment yields within a quantal description is the TDGCM (Regnier *et al* 2019, Zhao *et al* 2019, Younes *et al* 2019, Verriere and Regnier 2020). Here, a major difficulty is the determination of a proper manifold of states which usually consists of an ensemble of quadrupole and octupole constrained HFB solutions. While this description of quantum collective dynamics can treat tunnelling, it fails to include diabatic aspects of the dynamics close to scission. Let us also mention recent TDHF (Simenel and Umar 2014, Goddard *et al* 2015, Goddard *et al* 2016), TDHF + BCS (Scamps *et al* 2015, Scamps and Simenel 2018) and TDHFB (Bulgac *et al* 2019a) studies of fission. In these cases, the initial configurations for the time-dependent calculations are generated by constrained calculations at some elongation beyond the outer turning point. These methods are well suited to investigate the role of shell effects at scission (Scamps and Simenel 2018, Scamps and Simenel 2019), and thus provide valuable guidance to more phenomenological models like the scission-point models discussed earlier in this section. As mentioned earlier in section 3.3, time-dependent theories will be challenged to reproduce the tails of the yield distribution, due to non-Newtonian Langevin trajectories, unless a mechanism equivalent to the random force of the Langevin equation is included (Aritomo *et al* 2014, Sadhukhan *et al* 2017). Moreover, the present formulation does not allow for the treatment of quantum tunnelling.

All these state-of-the-art methods have their own strengths and weaknesses. Yet, they all rely on determining the probabilities to populate a set of scission configurations. A common feature in all these approaches is that the fragment yields are computed at scission, where the two nascent fragments still interact through the nuclear force, see section 7.1. As a result, estimates of particle number with projection methods, for example, become extremely sensitive to the condition that define scission configurations. Other observables such as energy sharing between nascent fragments, may not be relevant at this stage of the fission process. Methods should be developed to determine the yields of observables further away from scission.

Current methods have been mostly focussed on the yields associated with the mass, charge, and sometimes TKE of the fragments. To go beyond this simple picture, the challenge is to extend the space of configurations in the fission channel in order to be able to make quantitative predictions of correlated yields for these three observables, and eventually additional ones. The new observables of interest are typically the angular momentum and parity of the nascent fragments.

Finally, the prediction of fission yields is essential for a correct description of *r*-process nucleosynthesis and superheavy elements. It would, therefore, be important to carry out systematic large-scale calculations of fission yields in regions of the nuclear chart far from the valley of stability. While such large scale calculations present a serious challenge for computationally intensive models of fission dynamics, some recent progress in this direction has been reported in Giuliani *et al* (2018), Lemaître *et al* (2018), Giuliani *et al* (2019), Rodríguez-Guzmán *et al* (2020).

7.3. Number of particles in fission fragments

The estimation of $Y(Z, A)$ is usually based on the assumption that the probability density of the mass and charge of the fragments associated with a Bogoliubov wave function is Gaussian.

However, in order to describe the odd–even staggering seen in charge distributions more refined methods are required.

In the MM DDD approach, the odd–even effect in fission yields can be attributed to the pair-breaking effect (Mirea 2014). In order to assign a particle number to a pre-fragment in the vicinity of the scission configuration, a condition has been introduced in Mirea (2011) based on the position of the neck. A similar approach to particle number identification was proposed in the DFT approach of Younes and Gogny (2011) using the unitary transformations on the total wave function aiming at maximising the localisation of pre-fragments.

Even earlier, a method has been proposed in Simenel (2010) to estimate the exact probability distribution of mass and charge in a nascent fragment created in microscopic models by introducing the particle-number projection for fragments. This method has been applied to determine the transfer probabilities of nucleons during collision reactions and then generalised to superfluid system (Scamps and Lacroix 2013) with the use of the Pfaffian method (Robledo 2009), and applied to fission (Scamps *et al* 2015) in TDHF + BCS, thus showing that the odd–even effects can be described with the mean-field dynamics. As discussed in section 3.12.1, these distributions are affected by the lack of one-body fluctuations and correlations (e.g., between mass and charge distributions). As shown in Simenel (2011), Williams *et al* (2018), Godbey *et al* (2020), the latter can be recovered to some extend for symmetric systems using the TDRPA (Balian and Vénéroni 1984).

It will be interesting to couple this approach with configuration-mixing methods and semi-classical descriptions of the fission process. One should also go beyond the approximation of identical occupation of time-reversed canonical HFB states assumed in Verriere *et al* (2019) to see whether the proper blocking of one-quasiparticle states in odd–*A* nascent fragments, associated with breaking of time reversal symmetry, is important for the description of odd–even staggering of fission yields.

7.4. Energy sharing

Most of the energy released in fission appears in the form of TKE of the fission fragments. Hence, a direct inverse correlation exists between TKE and their total excitation energy available for prompt neutron and gamma emission. Moreover, the distribution of TKE directly influences the prompt neutron multiplicity distribution, which has been measured in a few cases and is important in transport simulations of selected classes of integral experiments.

Once the nascent fragments are separated at scission, the Coulomb repulsion is transformed into kinetic energy. As indicated in section 3.8, however, different models predict different values for the collective kinetic energy at scission. It is typically a few MeV in TDDFT and ranging from zero to 20 MeV in various transport treatments. From a theoretical point of view a tolerance of 20 MeV, representing about 10%–15% relative uncertainty, might be deemed acceptable. However, a change of TKE by that much would significantly change the multiplicity of evaporated neutrons (by about two) and it is therefore an important challenge to fission theory to improve on the calculation of TKE.

The available total excitation energy in fission fragments can be calculated from the energy balance in a fission event, knowing the masses of the fissioning system and of the fission fragments, once those are determined via a chosen theoretical model, or extracted from systematics of experimental data. For any model that does not fully separate the fission fragments, the extraction of the energy sharing will be subject to large uncertainties, as energy can flow from one pre-fragment to the other through the neck, and in close proximity the nascent fragments exchange energy via Coulomb interactions. Moreover, the nascent fragments are generally distorted relative to their equilibrium shapes and the associated distortion energy will be converted to additional primary fragment excitation energy, thus affecting the resulting energy sharing.

Guidance on excitation energy partitioning is necessary for simulating neutron and photon emissions when the total excitation energy in the fissioning system increases (as in the case of fission induced by fast neutrons). The only indirect observable related to the excitation-energy sharing is the average number of neutrons per fission event as a function of mass, but the data beyond thermal neutron-induced fission and SF reactions are scarce. The results of average neutron multiplicity measurements as a function of mass for significantly different excitation energies in the fissioning systems, suggest that with increasing energy in the fissioning (actinide) system, most of the extra energy is deposited in the heavy fragments (Müller *et al* 1984, Naqvi *et al* 1986).

It has to be emphasised that the process of energy sharing poses an interesting and nontrivial question: does the energy sharing occur in the condition of thermal equilibrium that has developed between nascent fragments? In this case, the details of the process of neck formation and subsequent fracture would be of secondary importance, and only the density of states associated with each of the nascent fragments would play a role. On the other hand, if equilibrium is not reached during the saddle-to-scission evolution the details of the splitting process will be crucial. This issue is still not resolved. Namely, the TDDFT method, which has recently been used to parameterise the energy dependence of the excitation-energy sharing, predicts neutron multiplicities as a function of mass in agreement with experimental observations (Bulgac *et al* 2019a, Bulgac *et al* 2020). At the same time, an approach that models the excitation-energy sharing statistically on the basis of the microscopic level densities within a Brownian shape evolution framework, was also able to reproduce the experimental trend (Albertsson *et al* 2020).

7.5. Quantum entanglement

SF of even–even nuclei is a process by which a 0^+ quantum system decays into two excited nuclei which eventually, after prompt neutron and photon emission, turn into two product nuclei in their ground states, moving apart with opposite momenta. In this sense, the process is analogous to the emission of two electrons from a singlet state, with the additional complication that in fission, neutrons and gamma rays are emitted at or beyond the scission point.

The fission process conserves quantum numbers and, therefore, those that characterise the initial state, such as particle number (Bulgac and Jin 2017) and angular momentum, must be shared among all particles and quanta in the exit channel. For example, neglecting neutron emission, the final state would be a superposition of states of the two fragments with numbers of protons and neutrons in one fragment complementing those in the other fragment, so that they add up to the number of protons and neutrons of the initial fissioning nucleus. The particle numbers of the fragments are therefore entangled, and a measurement in one fragment collapses the information about the particle numbers in the other fragment.

The same is true for the measurement of γ rays, which are characteristic of a given nucleus and thus uniquely define the other fragment. Summing up the angular momenta of gamma rays emitted from one primary fragment collapses the information about the angular momentum of the other fragment in the exit channel. In the same way the angular-momentum polarisations of the two fragments are also entangled. The real question is whether these effects are ultimately important for experiment? Can they be observed at all? When and how does decoherence of this entanglement occur? Fission fragments may represent a unique opportunity to explore quantum entanglement of mesoscopic systems, that is, they can be the closest realisation of the Schrödinger cat phenomenon (Dobaczewski 2019).

7.6. Quantum numbers

An essential ingredient in the microscopic description of fission is the PES, constructed in an intrinsic frame and including pairing correlations in the BCS or HFB approximations, see section 3.2.1. Both of these break symmetries of the underlying Hamiltonian, and their restoration yields additional contributions to the PES; see discussion in section 6.1.

The restoration of particle number has a relatively small effect on the PESs in actinide nuclei, which are far from closed shells (Bernard *et al* 2019). However, it may have a significant impact on the ATDHFB or GCM inertias that determine the collective Hamiltonians; see section 3.10. In particular, extensive studies are needed in two specific areas. First, one should consistently calculate the PES for symmetry-restored wave functions in the case of particle number projection, possibly by including variation after projection to determine the intrinsic states. Second, and perhaps most important, is the development of a consistent theory of collective inertias for the symmetry-restored wave functions. Recent developments in the description and manipulation of particle number projected HFB states (called antisymmetrized germinal power in the quantum chemistry literature) (Dukelsky *et al* 2019) could potentially lead to a particle-number-projected ATDHFB theory.

The angular momenta of fragments is an important element that determines neutron yields and other decay properties (Wilhelmy *et al* 1972). Given a mean-field description of the nucleus and the knowledge of its quasiparticle excitation energies, current theoretical tools can be used to calculate the angular momentum content of the fragments. There are two components to the angular momentum of the newly formed fragments: non-collective and collective.

The non-collective angular momentum is carried by the quasiparticles in the pre-scission configuration that are transferred to the post-scission nascent fragments under diabatic conditions. They will end up in one or the other nascent fragment, depending on the evolution of the corresponding orbitals with elongation; see Bertsch *et al* (2019a) for an example of this transition. Their angular momentum is conserved, allowing one to estimate its contribution to that of the nascent fragment. The collective angular momentum arises because of the deformation of the compound nucleus. This component can be calculated by well-known projection techniques used to compute rotational bands in deformed nuclei. The only difference in the case of the fissioning system is that scission also affects the angular momentum of the system with respect to the orientation of the fission axis. The collective contribution to the angular momentum of the nascent fragments about the fission axis vanishes. As a result, the distribution of gamma radiation in the subsequent cascade will be anisotropic with respect to this axis (Bertsch *et al* 2019b). In fact, this anisotropy has been observed in SF, and a systematic measurement would provide an invaluable test of our overall understanding of the dynamics at the scission point.

There can be additional angular momentum generated as the pre-fragments separate, due to higher multipole components of the Coulomb field between them, see Bertsch (2019). It is, in fact, straightforward to calculate the effect of the electric quadrupole field on the post-scission nascent fragments, given their deformations and their initial separations. It would therefore be useful to have this information available when reporting fission calculations going through the scission point.

7.7. Fragment de-excitation

Nascent fragments emerge with significant excitation energies and then primary fragments cool down via various decay modes resulting in particle emission (neutrons and photons from prompt and delayed emission as well as electrons and antineutrinos from β decays). In current phenomenological approaches, the neutron emission proceeds after the nascent fragments have

fully accelerated becoming primary fragments, whereupon they are treated as compound nuclei that de-excite via particle emissions.

In order to carry out simulations of those decay chains, it is necessary to know the initial states of the primary fragments, in particular their initial excitation energy, angular momentum, and parity. On the other hand, experimental information regarding the fission fragments can only be obtained after neutron emission. Hence, few experimental data can inform phenomenological models, and the microscopic models can play an important role in providing the necessary input for a large range of reactions. The angular momentum of the emerging fission fragments is an important quantity that sets the competition between the neutron and γ emission, and it has an important influence on a variety of photon observables, from prompt fission γ multiplicity to the prompt fission spectrum and correlations between emitted photons. To a lesser degree, it can also influence the delayed neutron and γ properties.

To reduce uncertainties, the angular momentum properties of the fission fragments should be investigated in a framework that allows the total separation of the nascent fragments. It has been demonstrated in TDDFT that scission is followed by a relaxation period in which the nascent fragments transition to a deformation of primary fragments that is close to the ground-state deformation (Bulgac *et al* 2019a), thereby increasing the energy available for emission.

Both γ and β decays of the primary fragments can be described using the QRPA, thus defining a consistent framework both for the entrance and exit channels, see section 5. Because β-decay half lives are long compared to those of γ decays, they generally can be assumed to occur from the fragment ground state, thus making a finite-temperature description of β decay unnecessary. But it is important to take into account that the β decays may generally populate excited states in the daughter fragment, which would then undergo their own emission chain before a subsequent β decay could occur. Consequently, γ decay should be investigated for each primary fragment as a prompt phenomenon (in principle in competition with but usually after neutron evaporation). β decay to the resulting ground-state fission products should also be investigated, including forbidden transitions of particular importance for neutrino studies.

8. Computational strategy

Microscopic modelling of nuclear fission is an example of a computational grand challenge (Young *et al* 2009, Bishop and Messina 2009, Carlson *et al* 2016). One reason is the complexity of the problems, whose solutions require advanced notions of linear algebra, group theory, analysis, computer science, etc. Another reason is the sheer amount of computing needed. While a single, static HFB calculation may take between a few minutes to a few days to converge on a single CPU, depending on the functional, the number of broken symmetries and the types of constraints, up to dozens of millions of such calculations would need to be performed to tackle some of the problems discussed in this document (large scale PESs, functional optimisations, time evolution, action minimisation, symmetry restoration). In this section, we discuss the various computational strategies that are currently available or should be explored in the future.

8.1. Computer codes for fission

There is a broad consensus that fission is not a problem that can be handled by a single code. Instead, the community should think of an ecosystem of different frameworks addressing different facets of the problem, for example, static versus time-dependent calculations. Since fission calculations are almost always characterised by the need to compute and manipulate very deformed configurations in heavy nuclei, this imposes specific requirements about the codes. In this section, we review some of the existing software and identify current gaps.

8.1.1. Brief review of available codes. A number of computer codes are available for modelling various aspects of fission dynamics. The most computationally intensive ones are those used for the calculation of HFB configurations and related quantities (inertias, energy overlaps, time-dependent evolution, etc). Two basic implementations of HFB/TDHFB solvers differ in the representation of the single-particle wave functions:

Space discretisation. This family of codes employs a finite volume, either in coordinate space or momentum space, that is discretised using a suitable mesh of points. Many different choices can be found in the literature, from the Lagrange mesh based on orthogonal polynomials (Baye 2015), to B-spline-based (Blazkiewicz *et al* 2005, Pei *et al* 2008), and adaptive wavelet-based methods (Pei *et al* 2014). Among the codes relevant for fission we mention: Sky3D (Maruhn *et al* 2014, Afibuzzaman *et al* 2018, Schuetrumpf *et al* 2018), and EV8 (Ryssens *et al* 2015b) (publicly available) as well as HFB-AX (Pei *et al* 2008), MADNESS-HFB (Pei *et al* 2014), MOCCa (Ryssens 2016), HFB-2D-LATTICE (Terán *et al* 2003, Blazkiewicz *et al* 2005), Skyax (Reinhard *et al* 2020), and the code of Jin *et al* (2017).

Basis expansion. This family of codes is based on an expansion of single-nucleon wave functions in a finite set of suitable basis functions. Most often this is a basis of the harmonic oscillator (HO) eigenfunctions. There have also been attempts to use the transformed HO basis states (Stoitsov *et al* 2003), or a two-centre HO basis for improving the description of elongated shapes (Dubray *et al* 2008). Some of the principal codes that use this representation for fission modelling are: HFODD (Schunck *et al* 2017) and HFBTHO (Perez *et al* 2017) (both publicly available,) as well as HFBaxial (Robledo 2010a, Robledo *et al* 2018), HFBTri (Robledo *et al* 2018), and HFB3 (Hashimoto 2013). The code HFB3 utilises a basis expansion for two Cartesian directions while employing a Lagrange mesh in coordinate space in the third. Two codes based on relativistic EDFs have recently been used in calculations of self-consistent mean-field configurations as input for modelling fission dynamics: DIRHB (Nikšić *et al* 2014) and MDC-RMF (Lu *et al* 2014).

The use of different representations determines the applicability of any given code. For instance, all numerical schemes can efficiently deal with zero-range (Skyrme-like) effective interactions; however, apart from implementations in spherical symmetry (Bennaceur 2020), mesh-based discretisation schemes have not been able to employ finite-range effective forces so far. On the other hand, basis-expansion methods have a long history of calculations with (among others) various Gogny interactions (Robledo *et al* 2018), Coulomb (Dobaczewski *et al* 1996), and Yukawa (Dobaczewski *et al* 2009) forces, by expanding the interaction into Gaussian form factors. Extensions to more general finite-range interactions have also been proposed (Parrish *et al* 2013).

For the time-dependent calculations of fission dynamics, only mesh-based methods have been used so far. They satisfy the demands of extreme deformations encountered at scission, and also allow the description of the nascent fragments beyond scission. While techniques exist to optimise the choice of basis states, mesh-based calculations have the advantage that their numerical precision is essentially independent of the nuclear deformation (Ryssens *et al* 2015a).

A major aspect of the difference between the two numerical schemes is the discretisation of the continuum. The first consequence of this is the treatment of pairing correlations since mesh- and basis-based methods give very different descriptions of positive-energy single-particle states. On the one hand, the coordinate representation takes correctly into account asymptotic properties of single-particle wave functions, but it becomes impractical and time-consuming

when dense single-particle states extending to high energies are included. This is required for a full HFB description of the coupling between quasiparticle and quasihole states (Dobaczewski *et al* 1984). On the other hand, basis-expansion methods can easily manage states of arbitrarily high energy, but fail to reproduce the spatial asymptotics of wave functions, and are thus not appropriate for the description of weakly-bound systems. In view of the importance of pairing for fission applications, see section 3.10, this situation is not satisfactory. One should note, however, that the practical importance of asymptotic properties or high-energy states in the continuum has not yet been evaluated for fission.

Another aspect is the treatment of finite-temperature calculations. When the nucleus is heated the Fermi surface becomes more diffuse and the statistical mixture includes contributions from quasi-bound and unbound single-particle states. While preliminary studies have been reported (Bonche *et al* 1984, Zhu and Pei 2014, Schuetrumpf *et al* 2016), the correct treatment of this degree of freedom is an open problem, see section 3.11. Nevertheless, as in the case of pairing correlations, we can already foresee that the applicability and performance of mesh-based and basis-based approaches will differ significantly.

Table 2 summarises the available codes for modelling deformed nuclei, their collective properties and fission dynamics. A few additional comments are in order: in the code Sky3D all spatial derivatives are evaluated using the finite Fourier transform method; the code of Hashimoto (2013) uses a Lagrangian coordinate-space grid in the direction of the axial-symmetry axis; the code of Jin *et al* (2017) uses a complete basis of single-particle states in the solution of the TDHFB; code SkyAx (HFODD) can implement constraints on axial monopole, quadrupole, octupole, and hexadecapole deformations (non-axial deformations up to multipolarity $\lambda = 9$) separately.

8.1.2. Development of new capabilities. Even if the codes listed above offer a high level of flexibility and great potentiality, we recommend the development of the following new computing capabilities.

Adaptive meshes. The specific issues of fission dynamics require that nuclear wave functions are computed also in regions where the nuclear density vanishes. For mesh-based implementations, uniformly spaced grids thus include discretised continuum represented by a large number of single-particle states, even at fairly low energies. For this reason, we recommend the development of a new-generation of mesh-based codes that will utilise non-uniform meshes, with lattice points concentrated in space regions where nuclear densities are non-negligible. This method would require self-consistent redefinitions of meshes depending on relative distances, deformations, and relative orientations of nascent fragments.

Adaptive bases. By definition, implementations that utilise two-centre HO bases describe only regions of space where densities are sufficiently different from zero. However, they require adaptive methods to self-consistently define bases corresponding to relative distances, deformations, and relative orientations of nascent fragments, as proposed in Dobaczewski (2019). We recommend the development of the corresponding HO-basis codes. Another direction is to use the multi-resolution techniques with a multi-wavelet basis as in Pei *et al* (2014).

General symmetry breaking. The concept of spontaneous symmetry breaking is crucial for a mean-field description of atomic nuclei, but it has not been exploited to its full capabilities yet. Even the most ambitious fission studies to date consider only configurations that still maintain certain self-consistent symmetries. In particular, time-reversal breaking configurations, needed for the description for odd and odd–odd nuclei as well as high-spin physics

Table 2. Summary of deformed HFB and TDHFB solvers. RHB stands for relativistic HFB. References to codes: [1] (Reinhard *et al* 2020), [2] (Maruhn *et al* 2014, Afibuzzaman *et al* 2018, Schuetrumpf *et al* 2018), [3] (Ryssens *et al* 2015b), [4] (Pei *et al* 2008), [5] (Pei *et al* 2014), [6] (Ryssens 2016), [7] (Jin *et al* 2017), [8] (Kim *et al* 1997, Simenel 2011, Scamps and Lacroix 2013), [9] (Sekizawa and Yabana 2016, Williams *et al* 2018), [10] (Umar and Oberacker 2005), [11] (Schunck *et al* 2017), [12] (Perez *et al* 2017), [13] (Robledo 2010a), [14] (Robledo *et al* 2018), [15] (Hashimoto 2013), [16] (Nikšić *et al* 2014), [17] (Lu *et al* 2014).

Coordinate space representation			
SkyAx	[1]	2D axial	Static CHF + BCS
Sky3D	[2]	3D Cartesian	CHF + BCS/TDHF
EV8	[3]	3D Cartesian	Static CHF + BCS
HFB-AX	[4]	2D axial, B-splines	Static CHFB
MADNESS-HFB	[5]	3D wavelets	Static HFB
MOCCa	[6]	3D Cartesian	Static CHFB
LISE	[7]	3D Cartesian	HFB/TDHFB
TDHF3D	[8]	3D Cartesian	TDHF/TDRPA/TDHF + BCS
3DTDHF	[9]	3D Cartesian	TDHF/TDRPA
VU-TDHF3D	[10]	3D Cartesian	TDHF (density constraint)
Basis expansion			
HFODD	[11]	3D HO	Static CHFB
HFBTHO	[12]	2D axial HO	Static CHFB
HFBaxial	[13]	2D axial HO	Static CHFB
HFBTri	[14]	3D HO	Static CHFB
HFB3	[15]	2D HO $\otimes$ 1D mesh	(TD)HFB
DIRHB	[16]	3D HO	Static C RHB
MDC-RMF	[17]	2D axial HO	Static C RHB

and multi-quasiparticle configurations, are not included in most available computer codes. To the best of our knowledge, HFODD and Sky3D are the only publicly available codes that include the degrees of freedom necessary for this type of studies.

GCM with time-odd momenta. Along the same line, an extension of current GCM codes to include time-odd collective momenta presents an interesting challenge. In addition to the implementation of time-reversal symmetry breaking, and the development of the actual GCM, this would also require the capability to consistently construct and constrain the relevant conjugate momentum operators.

Overlaps and kernels. Both GCM and projection methods require multi-reference calculations, that is, determination of overlaps and matrix elements between different paired or unpaired product states. In addition to possible problems related to the density-dependence of the interaction (Dobaczewski *et al* 2007, Lacroix *et al* 2009, Bender *et al* 2009, Duguet *et al* 2009, Robledo 2010b, Sheikh *et al* 2019), such calculations always require a higher degree of symmetry breaking than those for the corresponding single-reference implementations. For example, restoration of the particle symmetry or 3D rotational symmetry implies the time-reversal or simplex symmetry breaking, respectively, even if the single-reference states that are subjected to projection conserve these symmetries. Therefore, it is recommended that new codes are initially developed with a maximum degree of

symmetry-breaking capabilities, and then accelerated by implementing conserved symmetries in single-reference calculations. This will ensure that they are automatically portable to multi-reference frameworks.

Matrix elements. To implement K-matrix reaction theory for fission rates, as discussed in section 3.9, the suite of computer programs should be augmented with routines that calculate effective Hamiltonian matrix elements between arbitrary CHF and CHFB configurations. Also, the calculation of decay widths require including momentum operators in the set of constraining fields in the CHF and CHFB codes.

TDDFT, TDGCM, ATDDFT, and QRPA codes. We recommend building new-generation codes for fission dynamics by directly implementing the capabilities of the TDDFT, TDGCM, ATDDFT, and QRPA methods. For example, implementations built on HO bases, proposed in Dobaczewski (2019), can be ported to the time-dependent adaptive bases for TDDFT, or to the iterative solutions of the ATDDFT and QRPA methods.

Mesh-based codes for non-local EDFs. Since it is unlikely that higher accuracy of the calculated nuclear observables can be obtained using local EDFs (Kortelainen *et al* 2014), current developments are focussed on new-generation non-local EDFs. As discussed above, codes based on the HO basis are capable of treating such functionals fairly efficiently. It is, therefore, of paramount importance to develop algorithms for implementing the same capabilities in mesh-based codes. This is certainly a far-reaching goal; presently with no clear ideas on the direction to take. Nevertheless, we recommend that, because of its fundamental importance, a substantial effort should be devoted to attacking this problem.

Algorithmic improvements. All these developments recommended above depend on the efficient and robust generation of self-consistent mean-field solutions with many constraints. Constructing large numbers of these configurations is extremely demanding both in CPU time and in the time required to diagnose convergence issues. Besides the second-order gradient method (Robledo and Bertsch 2011), advanced algorithms from the field of non-linear optimisation have been introduced to accelerate the convergence of self-consistent iterations (Baran *et al* 2008, Ryssens *et al* 2019); the potential for further developments could be far greater. Supervised or deep learning techniques could also present significant opportunities to, e.g., optimise basis parameters for better numerical accuracy, perform real-time diagnostic about convergence, or provide good emulators of theoretical models (Lasseri *et al* 2020).

High-performance computing. Already in the late 2000s, nuclear fission was recognised as a scientific grand challenge justifying the development of exascale computer systems (Young *et al* 2009, Bishop and Messina 2009, Carlson *et al* 2016). Many of the various recommendations discussed in this document, from large-scale PESs with many degrees of freedom, to the coupling between TDHFB and TDGCM dynamics, will require the power of such facilities. Yet, this will require a serious effort by the community to modify, or re-factor, their codes in order to adapt to choices made at leadership computing facilities. Such choices include hardware architectures (GPU and hybrid chips, memory/core), software libraries (use of abstraction layers, more and more often in C++), or computing policies (limited runtime).

In conclusion, we recommend the development of numerical tools, which (i) target specific requirements of fission dynamics within the single-reference and multi-reference frameworks; (ii) are adapted to modern computing infrastructure; and (iii) build a common code base for fission theory. We advocate to increase the transparency associated with numerical choices by: (i) including a detailed description of numerical procedures in published studies (for benchmarking and an independent reproduction of the results); (ii) making codes publicly available

under Open Source license along with their long-term continuous maintenance within, e.g., a git repository; and (iii) writing the codes in a sufficiently modular fashion, so that new advances can be more easily adopted by the community.

8.1.3. Databases. As discussed in section 8.1.2, the computational cost to generate and store the mean-field configurations and their related quantities can be extremely high in the context of fission applications. At the same time, many applications only require 'integral' quantities related to these configurations. For example, computing SF lifetimes in the WKB approximation, or fission fragment distributions within the TDGCM + GOA framework, only requires the HFB PES and the collective inertia tensor. Let us assume for the sake of the argument a three-dimensional collective space with $200 \times 50 \times 50 = 500\,000$ points. Lifetimes, barrier penetrabilities, charge and mass distributions of the fission fragments can be computed merely from the knowledge of 1 scalar function of 3 variables (the energy) and a rank-2 tensor function of 3 variables (the inertia tensor). In our example, we would only need a grand total of 3.5×10^6 function values, which takes a very small amount of storage. By contrast, storing all the information about the HFB solution across the same PES would take up in excess of 1.6×10^{13} function values (assuming a $40 \times 20 \times 20$ box discretisation of 2000 HFB spinors). Having a database of such PESs for nuclei, different energy functionals (Skyrme, Gogny, relativistic, different pairing functionals, etc) and different DFT solver technologies would be very valuable to quantify theoretical uncertainties. Since the cost of generating a PES is high, it would also offer maximum leverage to our small community.

9. Recommendations and challenges

The purpose of this section is to summarise the main recommendations of this report that reflect challenges facing nuclear fission theory. The high-level recommendations, addressing the general challenges facing the field of microscopic nuclear fission theory, are listed in section 9.1. More detailed recommendations, pertaining to specific subareas, are listed in section 9.2. The ordering does not imply any priority.

9.1. High-level recommendations

General recommendations relevant to the field as a whole follow below. The numbers in brackets refer to key sections pertaining to individual recommendations.

Quantified input. Quantitative predictions require quantified input. It is essential to develop interactions and EDFs that are specifically tailored for the purpose of modelling fission. Of particular importance are the interaction components responsible for nuclear deformability and the pairing interactions that control the level of adiabaticity. It would be desirable to develop several quantified interactions/functionals for fission studies for (i) benchmarking purposes and (ii) to assess statistical and systematic uncertainties. Moreover, statistical calibration of interactions for fission should be carried out that would determine the sensitivity of parameters to key experimental constraints [sections 6 and 4].

Focus on essential ingredients. Considering limited resources, in order to maximise progress it is important to identify the essential ingredients in fission theory that require careful microscopic treatment and more robust ingredients that are necessary for a correct description of fission dynamics, but perhaps require less sophisticated modelling at the early stage of development. An example of essential ingredient is the PES. A more robust quantity is dissipation tensor; indeed many properties of predicted fission yields are found insensitive to large variations of the dissipation strength [section 4].

Modern theory extensions. There exist microscopic, yet greatly unutilised, extensions of current models of non-adiabatic large-amplitude collective motion that can be adopted to modern studies of nuclear fission. Many of those techniques involve algorithmic developments and significant computational capabilities. This includes: (i) description of fission trajectories in the full TDHFB manifold; (ii) inclusion of non-adiabatic couplings between many-body configurations; and (iii) consistent treatment of quantum and statistical fluctuations [sections 3–5, 8].

Comprehensive description. Fission is a complex phenomenon with a multitude of final channels and measured observables. In order not to be misled by a good agreement with limited classes of data, it is advisable to develop a comprehensive approach to fission observables. This is important because different elements of fission models are sensitive to different data. For instance, good reproduction of fission yields does not guarantee quality predictions of TKEs. In this context, priority should be given to modelling of measured quantities, not unobservables, which are primarily of theoretical interest [sections 7 and 2.2].

Access to quantum numbers. To be able to describe fission observables, a connection between models of fission dynamics based on the intrinsic-system concept, and the symmetry-conserved observables studied experimentally (particle number, angular momentum, parity) needs to be established. There are two possible avenues to achieve this goal. One is based on a reaction-theory approach that is explicitly formulated in the laboratory reference frame. Another way is by means of projection techniques. In both cases, many foundational developments are needed [sections 3 and 7].

Entrance channels. To model various kinds of fission, it is important to develop a unified description of initial states. At various instances of the fission phenomenon (from SF to fission induced by fast probes; from low-energy to high-energy fission), the entrance channel should be properly described. This includes the realistic modelling of compound nucleus for neutron-induced fission as well as specific nuclear states populated in photofission or β-decay. In the latter case, implementation of flexible QRPA methods (for any shape, for arbitrary multipole and charge-exchange channels, and indiscriminately for even–even, odd, and odd–odd systems) is recommended [section 5].

Computing. Future exascale computing ecosystems will offer a unique opportunity for microscopic modelling of nuclear fission. To achieve this goal, this report recommends the development of specific computing capabilities and launching a library of general-purpose fission software based on novel algorithms and programing that can efficiently utilise modern computing infrastructures. To this end, collaborations with computer scientists, applied mathematicians, and data scientists will be needed to (i) develop open-source, modular nuclear solvers and (ii) leverage high-performance computing and statistical machine learning [section 8.1].

Databases. Establish databases of microscopic fission output for further processing. This can include various HFB and TDHFB results (PESs, fission pathways, fission fragment yields and properties). Having computed multi-model fission data available will be essential not only for post-processing but also for benchmarking and uncertainty quantification [section 8.1.3].

9.2. Specific recommendations

A number of specific recommendations are proposed in the body of this report. The numbers in brackets refer to specific sections where individual recommendations can be found.

Microscopic tunnelling. In the studies of SF and low-energy fission, a part of collective motion proceeds through the classically-forbidden space. The most commonly used approach is that based on the CSE and a WKB approximation, in which the tunnelling rate is obtained from the collective action calculated along an effective one-dimensional trajectory. Limitations of this approach should be studied and, depending on the outcome, extensions explored. Those include: generalisation of the one-dimensional WKB treatment to several dimensions; increasing the number of collective coordinates; or other approaches to tunnelling, such as the imaginary-time method [section 3.6].

Classical aspects of TDDFT. Since TDHF equations emerge as a classical field theory for interacting single-particle fields, the TDDFT approach can neither describe the motion of the system in classically-forbidden regions of the collective space nor quantum fluctuations. In the context of tunnelling, one should determine the feasibility of arriving at instanton solutions to the TDDFT fission problem and develop methods to calculate the full ATDHFB collective inertia. As far as fluctuations are concerned, this problem shows up in too-narrow fission yield distributions predicted by time-dependent theories. A possible resolution to this problem lies in the stochastic mean-field approach that allows larger fluctuations in collective space [section 3].

Extend theory beyond even–even systems. Most microscopic calculations of nuclear fission pertain to even–even nuclei. It is therefore urgent to develop a consistent theoretical framework for the fission of even–even, A–odd, and odd–odd nuclei. This will require going beyond the usual blocking approximation to fully consider time-reversal symmetry-breaking effects. Odd–even staggering of fission yields is an example of a quantity that can be sensitive to such effects [sections 3 and 7].

Microscopic Langevin approach. Classical Langevin theory has been very successful in explaining many properties of fission products. To bridge it with microscopic fission frameworks, it is important to clarify the connections between microscopic TDHFB and TDGCM with dissipative theories—to make contact with Langevin-based approaches [sections 3.12 and 7].

Reaction-theory framework. An approach to fission based on reaction theory is useful, because it is explicitly formulated in the laboratory reference frame, which guarantees that the important quantum numbers are conserved. One should consider assessing the feasibility of developing a practical microscopic approach to fission based on the K-matrix reaction theory. It offers a completely different calculational framework for SF as well [section 3.9].

Generalised fission path. On the way from the entrance configuration to scission, the fissioning nucleus explores the continuum of trajectories in the collective space. Current approaches explore limited sectors of this space and hence it is essential to develop methods to search for optimum fission pathways in such a way that a blind exploration of the full multi-dimensional collective space is not required [section 4.1].

Generalised constraints. It would be very useful to go beyond simple constraining operators for which important configurations may be overlooked. Within the large family of density constraints, the technique that constrains the entire density distribution obtained in TDDFT is promising in that it provides a tight control of the shape. It naturally localises the system in the space of nuclear configurations, as does wave function constraints such as the K-partitioning. Also, constraints based on fission observables may be useful in the study of fluctuations [section 3.2.2].

Residual interactions. The ability to compute Hamiltonian matrix elements between configurations is essential for microscopic calculations of reaction theory, level crossing dynamics, and the dissipation tensor. This capability is already included for the pairing interaction in CHFB. However, the neutron–proton interaction is ignored in current codes except for its mean-field contribution [sections 3.9, 3.7 and 3.12.3].

10. Summary and conclusions

This topical review is unconventional: rather than presenting past achievements, it aims at reviewing future options for theory of nuclear fission. As we discussed in the introduction, numerous reviews and books that discuss experimental and theoretical aspects of nuclear fission exist (Schunck and Robledo 2016, Bertsch *et al* 2015, Andreyev *et al* 2017, Talou *et al* 2018, Schmidt and Jurado 2018, Krappe and Pomorski 2012, Younes *et al* 2019). The interested reader is encouraged to consult these references for more extensive and detailed information. The goal of the present work was to lay down our opinions on directions of future research in theory of nuclear fission. While this task is challenging, we found it useful to talk about research directions that seem to be promising and at the same time may be long overdue.

We will be most happy if our ideas are picked up by enthusiastic researchers working in this domain of nuclear physics, and even more, if they attract new talent into this area. Undoubtedly, many proposed directions will require concerted efforts of large collaborations, and we hope that this topical review will contribute to fostering those.

Beyond phenomenological modelling, the theoretical description of nuclear fission requires novel ideas on how to treat the incredible complexity of the phenomenon in a manageable and physically meaningful way. To be implemented, many of those ideas require advanced computations. In this document, we call for performing baseline work on developing quantified interactions/functionals for fission studies; identifying the essential ingredients in fission theory; utilizing extensions of current models of non-adiabatic large-amplitude collective motion; developing a comprehensive approach to fission observables; making connection between models based on the intrinsic-system concept and the symmetry-conserved observables; and for realistic modelling of the compound nucleus as well as of the specific nuclear states that form gateways to fission. Each and every one of these projects may in the future become a challenging research direction. Together, they may lead to a major advance of the field.

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ORCID iDs

Michael Bender https://orcid.org/0000-0001-8707-3410
Satoshi Chiba https://orcid.org/0000-0001-7123-7230
Jacek Dobaczewski https://orcid.org/0000-0002-4158-3770
Samuel A Giuliani https://orcid.org/0000-0002-9814-0719
Denis Lacroix https://orcid.org/0000-0002-6296-2112
Witold Nazarewicz https://orcid.org/0000-0002-8084-7425
Junchen Pei https://orcid.org/0000-0002-9286-1304
Jørgen Randrup https://orcid.org/0000-0002-7618-4876
Paul-Gerhard Reinhard https://orcid.org/0000-0002-4505-1552
Luis M Robledo https://orcid.org/0000-0002-6061-1319
Wouter Ryssens https://orcid.org/0000-0002-4775-4403
Nicolas Schunck https://orcid.org/0000-0002-9203-6849
Ionel Stetcu https://orcid.org/0000-0002-5271-2021
Paul Stevenson https://orcid.org/0000-0003-2645-2569
Sait Umar https://orcid.org/0000-0002-9267-5253
Marc Verriere https://orcid.org/0000-0002-0153-1212
Michał Warda https://orcid.org/0000-0001-6723-1020

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