MULTISCALE MODELS OF CRYSTAL DEFECTS

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1 Overview of the Field

The mathematical theory of solid mechanics has traditionally focused on the models of continuum mechanics, which is in stark contrast to the vast scientific literature employing atomistic models, particularly in the physics and materials science communities, to study material behavior. Only the past few years have seen the beginning of an effort to establish the mathematical foundations of atomistic models of solids, including the foundations of numerical algorithms and the connections to coarse-grained descriptions (e.g., continuum models).

Crystal defects play an important role in determining material parameters. For example, dislocations are the origin of plasticity; inclusions and other types of defects can ”pin” dislocations, and cause hardening. The modeling of crystal defects is a broad scientific field that spans many spatial and temporal scales, from quantum mechanical models of nuclei to effective continuum theories of plasticity; and many disciplines, including mathematical modeling, mechanics, and scientific computation. For this workshop we focused on the interplay between the discrete structure of defect cores and the elastic fields through which they interact with their environment, and the roles of mathematical analysis and numerical computations.

Over the past decade there has been increasing interest in the mathematical analysis community on atomistic multi-scale methods, starting from atomistic descriptions of materials. The focus of this research effort has been the rigorous derivation of effective continuum models from atomistic models. Some of the main achievements in this area include proofs of crystallization, rigorous understanding of the Cauchy–Born approximation, and rigorous asymptotic results on effective dislocation models.

In the numerical analysis community there has recently been much interest in the development and analysis of atomistic-to-continuum coupling methods. These are a class of numerical coarse-graining techniques used for the efficient atomistic simulation of material defects in large computational cells. There exists a wide range of techniques in this class, and the effort of numerical analysts has led to a clear picture of the key approximations made, the reliability of the various approaches, and the challenges that remain to be overcome.

Much of the rigorous analytical work has focused on the derivation of continuum elasticity from atomistic models. Even when defects are considered, the need for a detailed understanding of the discrete core structure is usually circumvented by making simplifying assumptions on the models. The stated aim of this workshop was to fill this gap and to begin a systematic study of the atomistic structure of crystal defects, by providing a platform for close interaction between engineering and materials science, numerical simulation, and mathematical analysis.

2 Recent Developments and Open Problems

The modelling and simulation of crystalline defects is a broad field. Here, we focus on some concrete areas of current activity in the mathematics community as well as scientific numerical methodologies. Yet, the techniques of numerical analysis are ideally suited to identifying the main sources of errors in such numerical simulations, thus identifying bottlenecks on where to focus new developments.

2.1 Numerical analysis of multi-scale methods

Atomistic and multi-scale simulation are indispensable components of modern materials science research, as is evidenced by the award of the 2013 Nobel Prize in Chemistry for the development of such simulation techniques. Until very recently there has been next to no mathematical foundation underpinning these techniques.

While there were a few earlier contributions, the numerical analysis theory of multi-scale methods began in earnest around 2008 with a number of papers appearing at the same time, from different groups. The focus has been on developing a rigorous theory of atomistic-to-continuum coupling methods, a paradigm case of a multi-scale scheme. Briefly, the idea is that a crystalline region containing a defects (or multiple defects) is modelled atomistically, while the surrounding crystalline bulk is treated by a continuum model. The key component in such a simulation is the "handshake" mechanism, the biggest difficulty being the transition from a non-local (atomistic) to a local (continuum) model. Such methods have been under development in the computational science community since the early 80's.

The numerical analysis theory has made some remarkable achievements: separation of the different sources of error (far-field boundary condition, continuum model, coarse-graining, and coupling) and characterisation and benchmarking of the different coupling mechanisms, identification of "universally stable" coupling mechanisms. All this has been achieved within a rigorous mathematical context. Further, the theoretical results have led to highly optimised formulations and prototype implementations with quasi-optimal convergence rates. See [1, 2] and references therein.

While challenging open problems remain in the field of zero-temperature atomistic/continuum coupling, much of the attention has recently turned towards two new frontiers: coarse-graining at finite temperature (see § 2.2) and coupling between quantum mechanics and molecular mechanics. The significant difficulty in the latter is that quantum mechanics is an inherently long-ranged theory which makes the non-local to local transition particularly challenging.

2.2 Coarse-graining of materials at finite temperature

While the extraction of continuum theories from deterministic discrete models is conceptually clear thanks to tools such as the Cauchy-Born rule the connection between the corresponding finite temperature systems and the continuum limits is less obvious. Finite temperature versions of standard tools such as the Cauchy-Born rule or stability are still in the process of development. As a result, many fundamental question are still awaiting mathematical treatment. Examples include the existence for solid phases at finite temperature, theoretical prediction of aging rates, and characterisation of thermodynamic parameters such as heat conductivity in terms of atomistic properties.

Current efforts concentrate mainly on static problems, key challenges are the characterization of nucleation energies and properties of the solid phases. Recent progress has been the result of the introduction of multiscale methods such as renormalisation groups, finite-range decompositions. Most results are of perturbative nature, e.g. the characterisation of elastic moduli.

The theoretical research efforts are complemented by the challenge to design efficient simulation strategies for materials at finite temperature. Key ideas in this direction are the quasi-continuum method which has been originally designed in the context of minimum energy problems. Recent ideas by Tadmor, Luskin, Perez,and Voter lead to generalisations of the methods so that finite-temperature cases can be simulated as well. This progress is the result of a careful localisation of the partition function. See, e.g., [6, 7] for early references in this field.

A relatively recent development is the idea to supplement the standard approach of deriving effective equations of motion based on theoretical analysis with methods from Machine Learning. Here the complex

model responses are treated probabilistically in the sense that one tries to automatise the construction of statistical models which predict the model responses.

2.3 Rigorous mathematical theory of dislocations

The characterisation of plastic material flow in terms of the microscopic material models is one of the holy grails in Material Science. The key step is the characterisation of the density and mobility of dislocations. Macroscopic laws like plastic harding are closely linked to dislocation mobility, which depends heavily on entanglement of the dislocation. Even a phenomenological statistical description is not available.

It is noteworthy that any discussion of dislocation structures is hampered by the presence of many length-scales. The first scale is given by the atomic structure of the core, and the energy contributions resulting from geometric properties such as curvature and climb. The second scale emerges from the spatial distribution of the dislocations, e.g. in the form of walls or networks. A third scale is introduced by the fact that plastic deformation itself will introduce internal structure. Well-known examples of this effect are elasto-plastic microstructures and strain-gradient plasticity.

The application of variational methods has recently lead to significant progress for static problems. It has been shown that (simple) dislocations can be interpreted as critical points in atomistic models for crystals [3]. This opens the possibility to characterize the strength of the pinning forces in terms of the depth and the geometry of the local energy well.

A related problem is the structure of dislocation walls (pile-ups) near grain boundaries, which is strongly influenced by the properties of the boundary, the interaction strength between the dislocations and the temperature. Progress has been achieved by several independent groups who managed to characterise the main patterns which are experimentally observed in terms of the scaling properties of the ground state energies.

Recently, much attention has been focussed on the study the microscopic evolution of dislocations. It would be highly desirable to derive standard macroscopic (rate-independent) evolution equation from discrete dislocation dynamics.

2.4 Simulation and Sampling with Molecular Dynamics

Molecular dynamics (MD) offers a robust and clear methodology for exploring a variety of physical systems at, for example, constant energy or temperature. MD models can retain full atomistic detail or be coarse grained. Up to the choice of physical approximations, their simulation output can be interpreted as, next to a laboratory experiment, the gold standard against which other methods should be compared. MD simulations allow practitioners to see how individual realizations of the system evolve and respond to thermal fluctuations and external forcing, and to sample equilibrium distributions, allowing for the computation of thermodynamic quantities. Important thermodynamic quantities include reaction rates for both defect migration in crystalline structures and changes of conformations in molecules.

Though simple to implement, the computational cost of MD often renders it impractical for either exploring the evolution of the system or computing thermodynamic quantities. Physical systems are often ripe with metastable regions in configuration space. When the system enters such a region, it may take a relatively long time to exit it, only to enter some other metastable region. For comparison, the typical time step in an MD simulation is that of a femtosecond, but the escape from a metastable region could be as much as a nanosecond. At the same time, interesting physical changes in the system might require transitions through many such metastable states, with time scales of microseconds or longer. For computing thermodynamic quantities, many such metastable regions must be visited to accurately sample the equilibrium distribution.

Over the years, there has been significant effort to develop approximations and algorithms that overcome metastability. One of the most celebrated such approximations is Transition State Theory (TST), which is robust in the case that the temperature of the system is sufficiently low and/or the energy barriers between states is sufficiently high. Using harmonic approximations, TST allows for the estimation of reaction rates amongst metastable regions which can form the basis of a kinetic Monte Carlo (KMC) model. However, not all systems have adequate scale separation for the harmonic approximation to hold, putting limitations on its applicability. Additionally, KMC models, based on TST, cannot capture correlated events in an atomistic system, such as the rapid transition over multiple energy barriers due to inertia.

A variety of other algorithms have appeared in the last two decades, including accelerated molecular dynamics, Wang-Landau sampling, nested sampling, adaptive KMC, Markov state models, and milestoning, which aim to improve upon TST. These methods are the result of decades of experience by MD practitioners and their physical intuition, along with some of the ideas that originate in TST. While these have allowed users to explorer larger systems, on longer time scales, the grand challenge remains simulating high dimensional systems over extended (laboratory) time scales.

Recently, an effort emerged on the part of mathematicians, particularly numerical analysts, applied probabalists, and scientific computing specialists, to build a rigorous, mathematical, foundation for coarse-grained dynamics and sampling schemes; see e.g. [4, 5].

3 Presentation Summaries

We had presentations on a wide range of topics related to the modelling, simulation and analysis of crystalline defects, with considerable overlap between speakers and topics:

- Numerical analysis of multiscale schemes: B. Vankoten, A. Shapeev, A. Binder, D. Trinkle, F. Legoll
- Models: G. Csanyi, P. Vorhees
- Temperature, free energy, Hot-QC:: A. Shapeev, D. Perez, P. Vorhees, C. Reina, F. Legoll
- Electronic structure aspects: E. Cances, F. Nazar, D. Trinkle, G. Csanyi
- Sampling, Stochastic homogenisation, variance reduction: G. Simpson, V. Ehrlacher, W. Minvielle, X. Blanc
- Analytical structure of defects: A. Garroni, F. Nazar, B. Vankoten, B. Schmidt, A. Binder
- Dislocation modelling: A. Garroni, C. Hall, D. Trinkle, P. Vorhees

We summarize all talks in alphabetical order:

Andrew Binder spoke about the Surface Cauchy-Born Method, an inexpensive multiscale technique for modelling surface effects. Surface effects can play a significant role in the determination of material properties on smaller scales. Despite the fact that surface effects are most influential in smaller systems, the systems may still be large enough that simulating the system atomistically will be computationally infeasible. The surface Cauchy-Born method was designed to efficiently model such systems and improve upon the regular Cauchy-Born method by better capturing surface effects. Binder showed the striking result that, while from a numerical analysis perspective, there is no reason to suspect improved accuracy of the SCB model, however, that there is a small physical parameter with respect to which the method does improve over classical Cauchy–Born.

Xavier Blanc spoke about elliptic problems in homogenization of periodic structure with defects. He presented an approach to approximate both at the coarse and fine scale the solution to an elliptic equation with oscillatory coefficients when this coefficient consists of a ”nice”, say periodic (the crystalline environment), function that is locally perturbed (the defect). The approach is based on computing a local defect profile given as the solution to an equation similar to the corrector equation in classical homogenization, but it is now posed in an infinite domain. The well-posedness of that equation were explored in various functional settings depending upon the locality of the perturbation, and decay estimates on the corrector were shown.

Eric Cances gave an introductory talk on electronic structure density functional theory for crystals with local defects. He started by presenting some simplified electronic structure models, Thomas-Fermi-Weizsäcker and reduced Hartree-Fock, as stepping stones towards the commonly employed Kohn-Sham density functional theory and the Hartree-Fock model, and surveyed the state of the art in their mathematical theory. He then presented analyses of situations with defects, both the case of a single defect and of a random distribution of local defects. For example a striking result is that the TFW model cannot model charged

defects. Cances concluded by mentioning open problems in this field including, e.g., the treatement of dislocations, or random defects with Coulomb interaction.

Gabor Csanyi presented the construction of highly accurate interatomic potentials using machine learning techniques. The most significant difficulty in extending quantum mechanical simulation techniques to larger length and time scales is that all exact formulations of quantum mechanics are non-local. Indeed it seems that the fundamental difference between the simplest semi-empirical quantum mechanical model (e.g. Tight Binding) and the most complicated classical model (at least for insulators) is that the quantum model involves some global operation over the entire system, like diagonalizing the whole Hamiltonian. Great strides have been made in making this less and less painful, principally by taking advantage of the sparse nature of the Hamiltonian and the density matrix, which can be considered to be a form of weak locality of the quantum model. However, it has long been known (indeed universally assumed and implicitly taken advantage of), that in most systems, there is a much stronger locality, namely that the forces, trajectories and general properties of an atom are not very dependent on the configuration of atoms far away. This motivates the construction of "interatomic potentials". These are mostly made by trial, error and guesswork. The GAP technique, which Csanyi presented, created interatomic potential automatically and rigourously using only the quantum mechanical data itself as input together with reasonable and universal assumptions about the smoothness and locality of the potential energy surface.

Virginie Ehrlacher discussed the approximation of effective coefficients in stochastic homogenization using a boundary integral approach. A very efficient algorithm has recently been introduced by Cances, et al. to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies on the clever use of a boundary integral formulation of the problem to solve. In her talk, Ehrlacher presented how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this end, she defined new approximate corrector problems and approximate effective coefficients and derived convergence results for this new formulation. Some numerical test cases illustrated the behaviour of this method.

Adriana Garroni gave an introduction to the mathematical analysis of dislocation models beginning from an atomistic description. She described an atomistic model for straight screw dislocations in different types of crystalline structure, for simplicity only treating anti-plane deformation. In this case the problem reduces to a two dimensional discrete model governed by a periodic potential. Garroni then study the asymptotic expansion of the energy of the system in the context of Γ-convergence as the lattice spacing tends to zero, where she identified the classical continuum elasticity model. Further, she then introduced a notion of effective gradient flow for the defects that account for the glide directions of the crystal.

Cameron Hall discussed formal asymptotic methods for connecting discrete models of dislocations with a continuum dislocation density model, focusing on the problem of dislocation pileup. A major challenge in multiscale modelling is to find the appropriate connections between the models that are relevant at different scales. This is especially difficult when trying to connect discrete models that track individual particles (whether they be atoms, discrete dislocations, or some other particle) with continuum models that deal with properties on a larger scale, such as deformation gradients and dislocation densities. Hall showed that a very effective way of approaching the problem of connecting these two scales is to use methods from classical asymptotics, such as the asymptotic approximation of sums using the Euler-Maclaurin summation formula, the method of multiple scales, and the method of matched asymptotics. In particular, he demonstrated how Euler-Maclaurin summation can be used to exploit regularity in the arrangement of particles to obtain the continuum model that is associated with a given discrete model. Then, he discussed how matched asymptotics can be used to analyse some cases where the assumptions required for Euler-Maclaurin summation break down, leading to discrete-scale boundary layer regions. From an applied perspective, these methods are useful because they demonstrate which physical interactions are important on which material scales, as well as giving a systematic framework for developing continuum models and canonical discrete models from a fundamentally discrete problem. From the perspective of mathematical analysis, these methods are also valuable because they give a way of finding ansatzes that can form the basis for establishing the convergence of energies via more rigorous methods.

Legoll, Frederic spoke about the calculation of defect formation (free) energy by a QCM-type approach. The formation free energy of defects is the difference between the free energy of an atomistic system with defects (computed in the canonical ensemble) and the free energy of the same system without any defects. This free energy difference, in the limit of asymptotically large systems, is a quantity of important practical interest, e.g., it determines the density of defects in the crystal. In practice, these quantities are difficult to compute as they require sampling extremely high-dimensional energy landscapes, and approximate models are normally employed. In this talk Legoll discuss the accuracy of a quasicontinuum type approach when computing these quantities.

William Minvielle spoke about variance reduction, via a control variate approach, for the homogenization of a random, linear elliptic second order partial differential equation set on a bounded domain in $\mathbb{R}^d$. The random diffusion coefficient matrix field $A(\frac{x}{\varepsilon}, \omega)$ is assumed to be uniformly elliptic, bounded and stationary ("periodic in law"). In the limit when $\varepsilon \to 0$, the solution of the equation converges to that of a homogenized problem of the same form, the coefficient field of which is a deterministic and constant matrix $A^\star$ given by an average involving the so-called corrector function that solves a random auxilliary problem set on the *entire* space. In practice, the corrector problem is approximated on a bounded domain Q_N as large as possible. A by-product of this truncation procedure is that the *deterministic* matrix $A^\star$ is approximated by a *random*, apparent homogenized matrix $A^\star_N(\omega)$. Minvielle therefore introduced a variance reduction approach to obtain practical approximations of $A^\star$ with a smaller variance in order to reduce the statistical error.

Faizan Nazar presented new results on locality of interaction in the Thomas-Fermi-von Weizsäcker electronic structure model. The TFW model is the paradigm example of an orbital-free density functional theory. The interaction between nuclei is obtained by solving a nonlinear PDE (eigenvalue problem) incorporating kinetic energy of the electron density and Coulomb interactions between electrons-electrons and electrons-nuclei. The model is inherently non-local; however, Nazar showed that the interaction between nuclei is *always* effectively local, i.e., it decays exponentially with distance between particles. He then applied this result to an analysis of crystalline defects in the TFW model.

Perez, Danny talked about the accuracy of kinetics in Coarse-Grained Molecular Dynamics. Multiscale methods that allow for a significant reduction of the number of dynamical degrees of freedom compared to conventional molecular dynamics are in principle ideally suited to simulate the long time dynamics of large systems. Indeed, the reduced computational cost associated with the integration of the equations of motion should enable the extension of the timescale horizon amenable to direct simulation. It is therefore important to assess the accuracy with which the long-time evolution is preserved upon coarse-graining. However, kinetics has of yet received much less attention than dynamics (e.g., wave reflection coefficients) or thermodynamics. In this talk, Perez showed how to quantify the error induced in Harmonic Transition State Theory (HTST) rates by the coarse-graining process. He then applied these results to the Coarse-Grained Molecular Dynamics (CGMD) formalism of Rudd and Broughton, providing both lower and upper bounds on the error on the HTST rates in terms of spectral characteristics of the atomistic and coarse-grained Hamiltonians and of the elastic response of the system. Within this framework he was able to identify and physically interpret the sources of error and present guidelines to determine the appropriate level of coarse-graining.

Celia Reina spoke about a self-consistent atomistic-phase field model for the study of Ge nanocrystallization. In her talk, Reine developed a new multiscale model for phase transformation in a heat bath at constant temperature. The model consists of a thermodynamically consistent phase field model that reproduces exactly the interface energetics and kinetics of atomistically computed crystallization fronts. As an additional feature, the interface thickness may be chosen arbitrarily large while preserving this exact atomistic-to-continuum coupling, in the case of flat interfaces. By extension this leads to controllable model errors in terms of interface curvature. This approach delivers a highly efficient multiscale computational model. As an application of this multiscale approach, Reina studied the interplay between nucleation and growth in the nano-crystallization of amorphous Ge. She demonstrated simple scaling laws between the mean radius of crystallized Ge grains, the nucleation rate and the time of crystallization.

Bernd Schmidt spoke about the passage from atomistic models to continuum theory in a crystal cleavage context. In his talk, Schmidt discussed the behavior of atomistic models in general dimensions under

uniaxial tension and investigated the system for critical fracture loads. He demonstrated a rigorous proof that in the discrete-to-continuum limit the minimal energy satisfies a particular cleavage law with quadratic response to small boundary displacements followed by a sharp constant cut-off beyond some critical value, a behaviour that had been conjectured (with some controversy), but only now rigorously proven. Moreover, Schmidt showed that the minimal energy is attained by homogeneous elastic configurations in the subcritical case and that beyond critical loading cleavage along specific crystallographic hyperplanes is energetically favorable. For some simplified situations he was also able to provide a complete characterization of the energy minimizing configurations

Simpson, Gideon described a relative entropy preconditioner for Markov chain Monte Carlo simulations. One of the challenges in using Markov Chain Monte Carlo methods to sample from a target distribution, such as the distribution of trajectories in a molecular dynamics problem, is finding a good proposal distribution. An ideal prior distribution would both be easy to sample from and have a high acceptance rate in the Metropolis step of the algorithm. This latter property ensures that the Markov chain will rapidly explore the configuration space under the target distribution. In this talk, Simpson presented work on functionalized Gaussian priors which are preconditioned to minimize the distance, with respect to relative entropy, to the target measure and showed exciting applications to path sampling.

Alexander Shapeev presented his recent ideas on evaluating the accuracy of (coarse-grained) defect calculations at finite temperature. While the analysis of accuracy for the calculation of crystalline defects at zero temperature has recently seen rapid development and major milestones, the corresponding finite temperature theory is wide open. In this talk, Shapeev presented a new and potentially fruitful approach to this issue. In order to continue to employ largely analytical (as opposed to probabilistic) methods he proposed to estimate the error of a coarse-grained calculation relative to an exact calculation by expanding both in termperature to arbitrary order. The errors in the expansion coefficents would then yield information on the coarse-graining error. He demostrated this principle on a non-trivial 1D example.

Dallas Trinkle discussed lattice Green function methods for electronic structure calculations in the presence of a dislocation. Flexible boundary condition for dislocations in bulk and in boundaries rely on accurate computation of the lattice Green function (LGF) from first-principles data. Previously, the lattice Green function for a perfect crystal was calculated directly from the bulk force constants, and applied to the relaxation of dislocations. However, that relies on the perfect LGF as an approximation to the LGF for the dislocation; even absent changes in the local force constants between atoms, a dislocation introduces a topological change in the connectivity of atoms (corresponding to a Burgers circuit). Trinkle showed a new numerical approach that accounts for the topology change of a dislocation, and estimated the error in previous calculations from the perfect LGF. He also discussed open or ill-understood issues connected to Green's functions for edge dislocations and challenges in obtaining optimal rates of convergence.

Brian Van Koten presented an error analysis of blended quasicontinuum methods for the simulation of defects at zero temperature. The BQC method is an atomistic/continuum coupling designed to simulate crystallographic defects. Van Koten presented an error analysis of the method valid for point defects in 2D or 3D crystals and also for straight screw dislocations. He showed a unique (in this field) "universal stability" result, that as long as the defect is stable in the atomistic model, BQC can simulate the defect accurately.

Peter Vorhees (Northwestern) spoke about the phase field crystal model, with particular applications to low-angle grain boundaries. Phase field crystal (PFC) models have been used to describe a wide range of phenomena from grain growth to solidification and dislocation motion in crystals. The strength of the method lies in its ability to follow the atomic scale motion over diffusive timescales. Peter Vorhees examined the evolution of the dislocation structure of a grain boundary and the local atomic displacements of atoms near the boundary during grain growth. He showed that the atomic scale structure of the boundary gives rise to qualitatively new grain growth kinetics as well as both grain rotation and translation. The grain translation is a result of the climb, glide, and interactions of the dislocations that comprise the grain boundary.

4 Scientific Progress and Outcome of the Meeting

The purpose of the meeting was not to solve major open problems, but to grow a new community and find common ground for collaboration, in particular across disciplines and subdisciplines, as well as targets to meet over the coming years. In this respect it was felt to be a resounding success by all participants.

Below are a representative (strict) subset of new ideas and collaborations that arose during this workshop:

- The talk of Vorhees served to show-case the potential of phase-field models for crystals. Here the objective is to derive approximations of single-particle marginal distributions related to the random process of the atomic positions at finite temperature. Phase field crystals are obtained by approximating of those marginal distributions by semi-linear elliptic equations. Thanks to an extensive mathematical theory of semi-linear equations it is possible to simulate the phase-field equations efficiently and thereby study the emerging properties of the underlying materials. A proper mathematical understanding of the derivation, simplification and simulation of phase field equations is still in its infancy. It is certain that the study of those questions will influence future developments in applied analysis.

- Dallas Trinkle's talk inspired a discussion to generalise the numerical analysis of atomistic/continuum coupling to QM/MM coupling schemes. He showed how even for relatively simple static problems (computing the equilibrium state of a dislocation) constructing a highly accurate QM/MM scheme is non-trivial. A further question that arose is how to optimally distribute computational resources. Further discussion between Trinkle and other participants have led to new research projects, and potential for future collaboration.

- Gideon Simpson's talk demonstrated how, in the case of path sampling, some of the challenges of sampling high-dimensional configurations can be overcome. This led to a discussion with Gabor Csanyi and others, on how to incorporate these techniques into sampling configurations (rather than paths). The conclusion of this discussion is that the seemingly canonical approach will not achieve this, but that some interesting technical questions must first be answered. There are plans for further collaboration.

- Gabor Csanyi's talk on the construction of highly accurate interatomic site energies raised the open problem of how to treat long-range forces (Coulomb and related) in this context. A concrete suggestion of Shapeev has led to a collaboration with plans for future implementation.

- Eric Cances presented the state of the art in the mathematical analysis of electronic structure of defects. Among the open problems he mentioned in his talk is the treatement of dislocations. Faizan Nazar's talk show-cased an improvement of a technique that will likely lead to tackling this in the near future.

- Shapeev's talk on defects in 1D chains at finite temperature triggered a half-day discussion between Shapeev, Theil and Schmidt. The result of the discussion was the insight that transfer-operator methods are equivalent to harmonic approximations provided the relevant profiles are known in advance.

- A particular highlight of the workshop was the chance encounter between Theil and Arnold Neumaier who participated in the parallel meeting on rigorous verification. Thanks to the discussion it became clear that computer aided constraint satisfaction methods can play an important role to determine the structure of atomistic defects. It was agreed to study the double kissing problem (Maximal number of neighbors of two touching spheres) in order to establish the feasibility of the concept.

- Comments from three attendant PhD students:

  "As a result of my participation in the BIRS workshop, I have gained a greater understanding of the physical models used in electronic structure theory. In particular, I have learned how they may be used in the context of analyzing defects such as for determining the decay rate of the change in the electronic density functions due to the defect. Finally, I have gained a greater understanding of other defects that are examined in this research field and their interest to material scientists."

  "At BIRS, I learnt about current work on treating defects, including approaches using homogenisation theory, work on understanding surface effects and the current state of considering defects in crystals

using Density Functional Theory, which is directly relevant to my area of research. I also had the opportunity to discuss my work and other related problems with the participants, which was very beneficial for me."

"The Banff workshop was a great place for me to learn about recent advances in material science; I specifically enjoyed contributions from the atomistic perspective. I am also very grateful to the organizers to give me the opportunity to present my work. I was delighted to meet with the leading scientists in the field. As a young researcher this is a great occasion to build new collaborations."

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