Modeling and Numerical Simulation in Mechanics and Materials Science

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2 Non destructive materials testing

In many situations we need to extract information on the inner structure of a medium from external indirect observations. Technology has provided many tools for different purposes: ultrasound, radar, seismic imaging... All of them are based on emitting some kind of wave which interacts with the medium under study, and is then measured at a set of receptors. Knowing the data recorded at the receptors and the emitted waves, we wish to reconstruct the internal geometry and/or material properties of the medium. We consider here two particular imaging set-ups for nondestructive testing of materials based on the use of acoustic and thermal waves.

2.1 Acoustic imaging

Let us consider a medium where a number of objects are buried. To simplify, we take the surrounding medium to be $\Omega_e := \mathbb{R}^2 \setminus \overline{\Omega}_i$, $\Omega_i \subset \mathbb{R}^2$ being the obstacle. Ω_i is an open bounded set with smooth boundary $\Gamma := \partial\Omega_i$ but has no assumed connectivity. There may be an unknown number of isolated components: $\Omega_i = \cup_{j=1}^{d} \Omega_{i,j}$ with $\Omega_{i,j}$ open connected bounded sets satisfying $\overline{\Omega}_{i,l} \cap \overline{\Omega}_{i,j} = \emptyset$ for $l \neq j$.

This configuration is illuminated by a time harmonic incident plane wave $U_{inc}(\mathbf{x}, t) = e^{\imath\omega t} e^{\imath\,\kappa^0\,\mathbf{x}\cdot\mathbf{d}}$ with frequency ω, wave number κ^0 and propagation direction $\mathbf{d}, |\mathbf{d}| = 1$. The incident wave interacts with the medium and the obstacles, generating a scattered wave and a transmitted wave. The total wave field is measured at detector locations placed on Γ_{meas}, far enough from the scatterers. Γ_{meas} may be a circle enclosing the obstacles in simple tests or a number of sites where receptors are located in more realistic reconstructions. In real experiments, the total field is known on the set of receptors Γ_{meas} for several incident directions $\mathbf{d}^j$.

The interaction between the scatterers, the medium and the incident radiation is described by a scalar transmission model for the acoustic wave. Since the incident field is time harmonic, the solution $U(\mathbf{x}, t) = e^{\imath\omega t} u(\mathbf{x})$ is time harmonic

too. The amplitud wave field $u = u_{inc} + u_{sc}$ in Ω_e and the transmitted amplitud $u = u_{tr}$ in Ω_i satisfy

$$\left|\begin{array}{ll} \nabla\cdot(\alpha_e\nabla u) + \lambda_e^2 u = 0, & \text{in } \Omega_e, \\ \nabla\cdot(\alpha_i\nabla u) + \lambda_i^2 u = 0, & \text{in } \Omega_i, \\ u^- - u^+ = 0, & \text{on } \Gamma, \\ \alpha_i\partial_{\mathbf{n}}u^- - \alpha_e\partial_{\mathbf{n}}u^+ = 0, & \text{on } \Gamma, \\ \lim\limits_{r\to\infty} r^{1/2}\left(\partial_r(u-u_{inc}) - \imath\kappa^0(u-u_{inc})\right) = 0, & r = |\mathbf{x}|, \end{array}\right.$$

with real parameters

$$\lambda_e(\mathbf{x}) \geq \lambda_e^1 > 0, \quad \lambda_i(\mathbf{x}) \geq \lambda_i^1 > 0, \quad \alpha_e(\mathbf{x}) \geq \alpha_e^1 > 0, \quad \alpha_i(\mathbf{x}) \geq \alpha_i^1 > 0.$$

The normal vector $\mathbf{n}$ points inside Ω_i. u^+ and u^- denote the limits of u from the exterior and interior of Ω_i respectively. $\partial_{\mathbf{n}}$ and ∂_r stand for normal and radial derivatives.

Knowing the values of the field u at a number of receptors, u_{meas}, for different incident waves we wish to obtain information on the objects buried in the medium. We can look for domains Ω_i which minimize an error in some sense. This leads to a constrained optimization problem: minimize

$$J(\mathbb{R}^2 \setminus \overline{\Omega}_i) := \frac{1}{2}\sum_{j=1}^{M}\int_{\Gamma_{meas}} |u^j - u^j_{\text{meas}}|^2 dl,$$

u^j being the solutions of M forward transmission problems with incident waves $u^j_{inc}(\mathbf{x}) = \exp(\imath\,\kappa^0\,\mathbf{x}\cdot\mathbf{d}^j)$. This functional depends on the design variable Ω_i through the transmission problems, which act as constraints.

The topological derivative of this cost functional helps to locate the objects.The topological derivative of the shape functional $\mathcal{J}(\mathcal{R})$ is defined as

$$D_T(\mathbf{x},\mathcal{R}) := \lim_{\varepsilon\to 0}\frac{\mathcal{J}(\mathcal{R}_\varepsilon) - \mathcal{J}(\mathcal{R})}{\mathcal{V}(\varepsilon)}, \qquad \mathbf{x}\in\mathcal{R},$$

where $\mathcal{R}_\varepsilon$ is $\mathcal{R}$ minus a ball centered at $\mathbf{x}$ with radius ε. $\mathcal{V}(\varepsilon)$ is minus the volume of the ball. In our case, $\mathcal{V}(\varepsilon) = -\pi\varepsilon^2$. Asymptotic expansions provide a result easier to implement [22, 24]: The topological derivative of the cost functional in $\mathcal{R} = \mathbb{R}^2 \setminus \overline{\Omega}$ is given by

$$D_T(\mathbf{x},\mathbb{R}^2\setminus\overline{\Omega}) = \sum_{j=1}^{M}\text{Re}\Bigg[\frac{2(\alpha_e(\mathbf{x})-\alpha_i(\mathbf{x}))}{1+\frac{\alpha_i(\mathbf{x})}{\alpha_e(\mathbf{x})}}\nabla u^j(\mathbf{x})\nabla\overline{p}^j(\mathbf{x}) + (\lambda_i^2(\mathbf{x}) - \lambda_e^2(\mathbf{x}))\,u^j(\mathbf{x})\overline{p}^j(\mathbf{x})\Bigg],$$

for any $\mathbf{x}\in\mathbb{R}^2\setminus\overline{\Omega}$ assuming the coefficients smooth. The forward field u^j solves the forward transmission problems with the j-th incident wave and $\Omega_i = \Omega$.

The adjoint field p^j solves

$$\left|\begin{array}{ll}
\nabla\cdot(\alpha_e\nabla p^j)+\lambda_e^2 p=(u^j_{meas}-u^j)\,\delta_{\Gamma_{meas}}, & \text{in } \mathbb{R}^2\setminus\overline{\Omega}_i\ ,\\
\nabla\cdot(\alpha_i\nabla p^j)+\lambda_i^2 p^j=0, & \text{in } \Omega_i,\\
(p^j)^- -(p^j)^+=0, & \text{on } \partial\Omega_i,\\
\alpha_i\partial_{\mathbf{n}}(p^j)^- -\alpha_e\partial_{\mathbf{n}}(p^j)^+=0, & \text{on } \partial\Omega_i,\\
\lim\limits_{r\to\infty} r^{1/2}\left(\partial_r p^j+\imath\kappa^0 p^j\right)=0, &
\end{array}\right.$$

with $\Omega_i=\Omega$. Here, $\delta_{\Gamma_{meas}}$ is the Dirac delta function defined on Γ_{meas}. Visualizing the topological derivative field for $\Omega_i=\Omega=\emptyset$ we find information on the objects: they are located at regions where the topological derivative is negative and large. An iterative procedure allows us to improve it [24, 30, 45]. Different conditions at the interface than transmission conditions, such as Dirichlet or Neumann can also be considered [31, 22] for 'hard' and soft' objects.

2.2 Damped waves and thermal imaging

Acoustic waves propagating in some media are subject to damping effects: the obey wave equations with damping terms. When the incident waves are time harmonic, their amplitude satisfies Helmholtz equations with complex wave numbers. Otherwise, the formulation follows similar lines a before. However, in this case one can mostly detect objects that are close to the surface. The resolution improves when we superimpose frequencies weighting their contributions [63].

A similar strategy can be applied to time dependent thermal waves [26], which solve transmission heat problems

$$\left\{\begin{array}{ll}
U_t-\kappa_e\Delta U=0, & \text{in } \mathbb{R}^N\setminus\overline{\Omega_i}\times(0,\infty),\\
U_t-\alpha_i\kappa_i\Delta U=0, & \text{in } \Omega_i\times(0,\infty),\\
U^- -U^+=U_{\text{inc}}, & \text{on } \partial\Omega_i\times(0,\infty),\\
\alpha_i\frac{\partial}{\partial\mathbf{n}}U^- -\frac{\partial}{\partial\mathbf{n}}U^+=\frac{\partial}{\partial\mathbf{n}}U_{\text{inc}}, & \text{on } \partial\Omega_i\times(0,\infty),\\
U(\,\cdot\,,0)=0, & \text{in } \mathbb{R}^N,
\end{array}\right.$$

Topological derivative methods allow us to approximate solutions of the inverse problem for such waves [26]. Combining with gradient methods, it is also possible to find, not only the object geometry, but also its material constants κ_i, α_i, see [46].

2.3 Electrical impedance tomography

The impedance imaging problem consists in producing an image of the electromagnetic properties of a medium by applying electric currents to its exterior surface and measuring voltages on it. The range of medical applications is wide, because different tissues have different electromagnetic properties. For example, we can think of monitoring for lung problems (embolies, clots, accumumation

of fluids) or blood flow (internal bleeding, heart function), screening for breast cancer, determining the boundary between dead and living cells, detecting temperature changes in hyperthermia treatments...

We want to reconstruct the admittivity γ inside Ω from measurements on the boundary. If we assume that Ω contains a number of inclusions $\Omega_{i,j}$, the admittivity γ is a piecewise function in Ω with discontinuities at the boundaries of the inclusions. We set $\Omega_i = \cup_{j=1}^{d} \Omega_{i,j}$ with $\Omega_{i,j}$ open connected bounded sets satisfying $\overline{\Omega}_{i,l} \cap \overline{\Omega}_{i,j} = \emptyset$ for $l \neq j$. The admittivity in the matrix $\Omega_e = \Omega \setminus \overline{\Omega}_i$ is γ_e. We define γ_i in Ω_i as $\gamma_i = \gamma_{i,j}$ in $\Omega_{i,j}$. To simplify, we assume γ_e to be known. To identify the inclusions from the recorded data, we can solve the optimization problem [40]

$$J(\Omega_i, \gamma_i) = \frac{1}{2} \int_{\partial\Omega} |u - V_{meas}|^2 dl$$

where u solves

$$\begin{cases} \nabla \cdot \gamma_e \nabla u = 0 & \text{in } \Omega_e, \quad \nabla \cdot \gamma_i \nabla u = 0 & \text{in } \Omega_i, \\ u^- - u^+ = 0 & \text{on } \partial\Omega_i, \quad \gamma_i \partial_{\mathbf{n}} u^- - \gamma_e \partial_{\mathbf{n}} u^+ = 0 & \text{on } \partial\Omega_i, \\ \gamma_e \partial_{\mathbf{n}} u = j & \text{on } \partial\Omega. \end{cases}$$

The unit normal $\mathbf{n}$ points outside Ω_e but inside Ω_i and u^- and u^+ denote the limit values of u on $\partial\Omega_i$ from outside and inside Ω_i, respectively. Topological derivative methods allow us to approximate solutions of the inverse problem for such incident waves [40]. Instead of electromagnetic signals, other methods monitor temperature recordings to locate unhealthy tissue.

2.4 Holography and microwave imaging

Digital in-line holography is a promising tool for high speed three dimensional (3D) imaging of live cells and soft matter. It can achieve high temporal (microseconds) and spatial (nanometers) resolution while avoiding the usage of toxic stains and fluorescent markers. Holograms are two-dimensional (2D) light interference patterns that contain information about the 3D positions and optical properties of an object or set of objects.

When the emitted light beams are time harmonic, that is, $\mathcal{E}_{\text{inc}}(\mathbf{x}, t) = \text{Re}[e^{-\imath\omega t}\mathbf{E}_{\text{inc}}(\mathbf{x})]$, the resulting wave fields also happen to be time harmonic $\mathcal{E}_{\Omega,\kappa}(\mathbf{x}, t) = \text{Re}[e^{-\imath\omega t}\mathbf{E}_{\Omega,\kappa}(\mathbf{x})]$ and the complex amplitude $\mathbf{E}_{\Omega,\kappa}(\mathbf{x})$ satisfies a stationary version of the time dependent Maxwell equations, the so-called forward problem:

$$\begin{aligned} \mathbf{curl}\,(\tfrac{1}{\mu_e}\mathbf{curl}\,\mathbf{E}) - \tfrac{\kappa_e^2}{\mu_e}\mathbf{E} = 0 \quad &\text{in} \quad \mathbb{R}^3 \setminus \overline{\Omega}, \\ \mathbf{curl}\,(\tfrac{1}{\mu_i}\mathbf{curl}\,\mathbf{E}) - \tfrac{\kappa_i^2}{\mu_i}\mathbf{E} = 0 \quad &\text{in} \quad \Omega, \\ \hat{\mathbf{n}} \times \mathbf{E}^- = \hat{\mathbf{n}} \times \mathbf{E}^+, \quad &\text{on} \quad \partial\Omega, \\ \tfrac{1}{\mu_i}\hat{\mathbf{n}} \times \mathbf{curl}\,\mathbf{E}^- = \tfrac{1}{\mu_e}\hat{\mathbf{n}} \times \mathbf{curl}\,\mathbf{E}^+, \quad &\text{on} \quad \partial\Omega, \\ \lim_{|\mathbf{x}|\to\infty} |\mathbf{x}| \left| \mathbf{curl}\,(\mathbf{E} - \mathbf{E}_{\text{inc}}) \times \tfrac{\mathbf{x}}{|\mathbf{x}|} - \imath\kappa_e(\mathbf{E} - \mathbf{E}_{\text{inc}}) \right| = 0, & \end{aligned}$$

where $\mu_i, \varepsilon_i, \kappa_i$ and $\mu_e, \varepsilon_e, \kappa_e$ are the permeabilities, permittivities and wavenumbers $\kappa^2 = \omega^2 \varepsilon \mu$ of the objects and the ambient medium, respectively. In biological media, $\mu_i \sim \mu_e \sim \mu_0$, μ_0 being the vacuum permeability. The signs $+$ and $-$ denote the values from outside and inside Ω. The vector $\hat{\mathbf{n}}$ represents the outer normal vector.

The imaging problem becomes [53] finding objects Ω such that the equation:

$$\mathbf{I}_{\text{meas}}(\mathbf{x}_j) = |\mathbf{E}_\Omega(\mathbf{x}_j)|^2, \quad j = 1, \ldots, N,$$

is satisfied. Alternatively, we can reformulate this equation as a constrained optimization problem: Find the global minimum Ω of

$$J(\mathbb{R}^3 \setminus \overline{\Omega}) = \frac{1}{2} \sum_{j=1}^{N} |\mathbf{I}_\Omega(\mathbf{x}_j) - \mathbf{I}_{\text{meas}}(\mathbf{x}_j)|^2.$$

Here, $\mathbf{I}_\Omega = |\mathbf{E}_\Omega|^2$ and $\mathbf{E}_\Omega$ is the solution of the dimensionless forward system. Ω is the design variable in this optimization problem. The stationary Maxwell system is the constraint. The true objects are a global minimum at which the cost functional vanishes. By topological derivative techniques [53, 55] we can obtain first guesses of the objects. We can also iterate to improve this information. However, the iteration usually stagnates far from the true results. We encounter the same situation with other 'gradient' methods, such as level sets or deformation contours. Instead, hybrid schemes combining topological derivative initialization and updates with iteratively regularized Gauss-Newton corrections are able to produce good reconstructions of the number of objects as well as their size, location and shape [59, 65]. Holography is an extreme case in which only one incident beam is used and we use limited aperture data. When information from multiple incident waves (incoming from different directions and recorded at detectors distributed through large enough angles) is available, the initial guesses provides by topological derivatives furnish already a good reconstruction from the start, see [62] for microwave imaging tests.

2.5 Uncertainty Quantification

The methods just discussed are deterministic. Given recorded data, deterministic methods seek objects which would produce data as close as possible to the recorded data. However, recorded data are always affected by noise, which reflects uncertainty on the measurement device and the problem formulation. Deterministic methods provide a solution for a realization of the noisy data. No information on how the solution can change for other realizations or what confidence can we have on the proposed solution is given. Bayesian formulations of the inverse problem are used to quantify uncertainty in the result [61].

Bayesian formulations consider all unknowns in the inverse problem as random variables. Given a recorded hologram $\mathbf{I}_{\text{meas}}$ we seek a finite-dimensional vector of parameters $\boldsymbol{\nu}$ characterizing the imaged objects. When we assume the

presence of L objects, $\boldsymbol{\nu}$ is formed by L blocks, one per object. Using Bayes' formula

$$p_{\rm pt}(\boldsymbol{\nu}) := p(\boldsymbol{\nu}|\mathbf{I}_{\rm meas}) = \frac{p(\mathbf{I}_{\rm meas}|\boldsymbol{\nu})}{p(\mathbf{I}_{\rm meas})} p_{\rm pr}(\boldsymbol{\nu}),$$

where $p_{\rm pr}(\boldsymbol{\nu})$ represents the prior probability of the variables, which incorporates our previous knowledge on them, while $p(\mathbf{I}_{\rm meas}|\boldsymbol{\nu})$ is the conditional probability or likelihood of observing $\mathbf{I}_{\rm meas}$ given $\boldsymbol{\nu}$. The solution of the Bayesian inverse problem is the posterior probability $p_{\rm pt}(\boldsymbol{\nu}|\mathbf{I}_{\rm meas})$ of the parameters given the data. Sampling the posterior distribution, we obtain statistical information on the most likely values of the object parameters with quantified uncertainty. Markov Chain Monte Carlo techniques provide a tool to extract and visualize such information [61]. Time dependent problems with time dependent wave constraints can be handled in a similar way [66, 69].

3 Mechanical behavior of modular proteins

Tissue elasticity in living organisms results from the extension and recoil of proteins fastened to rigid structures that move under force. Polyproteins or modular proteins, such as titin that plays an important role in muscle contraction, ubiquitin and other relevant proteins, comprise a number of repeated single protein domains joined by short peptide linkers. A simple version of tissue elasticity appears in most single-molecule experiments, like atomic force microscopy (AFM), in which a biomolecule is chained to rigid platforms whose motion is controlled. Force-clamp and length-clamp experiments provide information on the protein structure, and can be interpreted by means of simple mathematical models. This section is taken from [39, 44, 47, 49].

In real experiments, the tip of the cantilever can attach the polyprotein at any point. Therefore, the number N of protein monomers exposed to force varies between one and the total number of monomers. Let the monomer positions be x_j, $j = 1, \ldots, N$. The relative extensions of the monomers are $u_j = x_{j+1} - x_j$, $j = 1, \ldots, N$ and external forces $\pm F$ applied to the ends of the monomer chain produce a potential $-F \sum_{j=0}^{N} u_j = F x_0 - F x_{N+1}$. Thus these forces on the chain ends yield an equal effective external force F on each of the extensions u_j. The free energy of the jth monomer is $V(u_j; \delta_j)$, where $V(u; \delta)$ is a double-well potential whose minima correspond to the folded (enthalpic) and unfolded (entropic) states. The parameter δ can vary from monomer to monomer. The monomers are connected to their next neighbors by harmonic springs (the linkers) and they undergo Brownian motion in the liquid in which they are immersed. We assume that their inertia can be neglected and therefore that their dynamics is overdamped. The resulting model is as follows [49]:

$$\begin{aligned} &\gamma_j \dot{u}_j = F - V'(u_j; \delta_j) - k_{j+1}(u_j - u_{j+1}) - k_j(u_j - u_{j-1}) + \sqrt{2 k_B T \gamma_j}\, \xi_j(t), \\ &\langle \xi_j(t) \rangle = 0, \quad \langle \xi_j(t) \xi_l(t') \rangle = \delta_{jl} \delta(t - t'), \quad j = 1, \ldots, N. \end{aligned}$$

Here $V'(u;\delta) = dV(u;\delta)/du$, $k_j = k$ for $j = 1, \ldots, N+1$. As explained before, the force F provided by the AFM affects the effective potential of all monomers between the AFM tip and the platform equally. There are two possible experimental settings: (i) The force F is kept constant (force-clamp experiments); (ii) the total extension of the chain is controlled and kept constant or increased at a uniform rate(force-extension experiments). In case (ii), $F(t)$ is a new unknown that should be calculated. The boundary conditions for this chain are

$$u_0 = 0, \quad u_N = 0.$$

We assume that the monomers at x_1 and x_N rigidly follow the platform and the AFM tip so that $u_0 = u_N = 0$. For case (ii) we need to add the constraint that the total length of the monomer chain, L, be kept constant so that the following new equation holds:

$$\sum_{j=1}^{N} u_j = x_{N+1} - x_0 = L.$$

In force-extension experiments, $L = \mu t + \nu$, with a positive μ.

3.1 Folding and unfolding

In a typical force-clamp experiment, the force is first raised, kept at a large value until all domains become unfolded and then abruptly lowered to a smaller value. Immediately after the force increment, abrupt or stepwise unfolding of the polyprotein follows. On the other hand, after the force is lowered, refolding is similar for single module proteins and for homopolyproteins; the folding events do not show traces of sequential folding for polyproteins.

Assuming infinitely rigid springs connect the protein to AFM cantilever and platform, $u_0 = u_1$, $u_{N+1} = u_N$. At zero external force and temperature T, we use the effective potential:

$$\begin{aligned} V(u) &= U_0\left[\left(1 - e^{-2b(u-R_c)/R_c}\right)^2 - 1\right] \\ &\quad + \frac{k_B T L_c}{4P}\left(\frac{1}{1-\frac{u}{L_c}} - 1 - \frac{u}{L_c} + \frac{2u^2}{L_c^2}\right). \end{aligned}$$

It is a cubic, with three zeros, three of which are stable. Given F, the smallest $u^{(1)}(F)$ and largest $u^{(3)}(F)$ zeros represent the folded and unfolded state for each module. Folding and unfolding phenomena can be explained qualitatively and quantitatively in terms of pinning and depinning of fronts in this system [21].

3.2 Force-extension curves

As the polyprotein is pulled, one or more modules unfold at a typical force that measures its mechanical stability. It should be stressed that the unraveling

of a domain is a stochastic event and may occur in a certain range of forces. These *length-clamp* experiments deliver a sawtooth force-extension curve (FEC). Similar curves are obtained by stretching nucleic acids and other biomolecules. When the force extension curve is swept at a finite rate, stochastic jumps between folded and unfolded states may be observed, and the unfolding force increases with the extension rate.

A simple model of an oscillator coupled to Ising spins that undergo Glauber dynamics [37] in contact with a thermal bath could explain qualitatively many features of the force-extension curves measured in experiments with biomolecules [39]. DNA force-extension curves correspond to cycling at different rates the curves of the spin-oscillator first-order phase transition with the force as a control parameter. The spin-oscillator model is too simple to account for the sawtooth pattern observed in length-controlled experiments.

Studying stationary solutions of the model proposed above [44], we have a global constraint in the minimization procedure leading to the equilibrium values of the extensions. As a consequence, the force-extension curve has multiple branches in a certain range of forces. The stability of these branches is governed by the free energy: there are a series of first-order phase transitions at certain values of the total length, in which the free energy itself is continuous but its first derivative, the force, has a finite jump. This behavior is completely similar to the one observed in real experiments with biomolecules like proteins, and other complex systems. The effect of noise and unequal monomer presence are studied in detail in [49].

4 Graphene mechanics

Graphene is a two dimensional material with promising mechanical and electronic properties. Its lattice structure consists of carbon atoms forming a hexagonal lattice. Different types of defects alter the hexagonal structure, as well as the mechanic and electronic properties of the material as a consequence.

4.1 Dislocations and defects

Periodized discrete elasticity models can describe typical defects and their dynamics [25, 23], which can be explained in terms of dislocations.

Consider a planar hexagonal graphene lattice and ignore possible vertical deflections. In the continuum limit, in-plane deformations are described by the Navier equations of linear elasticity for the two-dimensional (2D) displacement vector (u, v),

$$\rho_2 \frac{\partial^2 u}{\partial t^2} = (\lambda + 2\mu) \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y},$$
$$\rho_2 \frac{\partial^2 v}{\partial t^2} = \mu \frac{\partial^2 v}{\partial x^2} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial y^2} + (\lambda + \mu) \frac{\partial^2 u}{\partial x \partial y},$$

where ρ_2 is the 2D mass density and λ and μ are the 2D Lamé coefficients ($\lambda = C_{12}$, $\mu = C_{66}$, $\lambda + 2\mu = C_{11}$).

At lattice level, we obtain a discrete elasticity model for the atom dynamics as follows. We consider a point A in the hexagonal lattice with coordinates (x, y). Its 9 (3+6) closest neighbours have coordinates

$$n_1 = \left(x - \frac{a}{2}, y - \frac{a}{2\sqrt{3}}\right),\ n_2 = \left(x + \frac{a}{2}, y - \frac{a}{2\sqrt{3}}\right),\ n_3 = \left(x, y + \frac{a}{\sqrt{3}}\right),$$
$$n_4 = \left(x - \frac{a}{2}, y - \frac{a\sqrt{3}}{2}\right),\ n_5 = \left(x + \frac{a}{2}, y - \frac{a\sqrt{3}}{2}\right),\ n_6 = (x - a, y),$$
$$n_7 = (x + a, y),\ n_8 = \left(x - \frac{a}{2}, y + \frac{a\sqrt{3}}{2}\right),\ n_9 = \left(x + \frac{a}{2}, y + \frac{a\sqrt{3}}{2}\right).$$

Let us define the following operators acting on functions of the coordinates (x, y) of node A:

$$\begin{aligned} Tu &= [u(n_1) - u(A)] + [u(n_2) - u(A)] + [u(n_3) - u(A)], \\ Hu &= [u(n_6) - u(A)] + [u(n_7) - u(A)], \\ D_1u &= [u(n_4) - u(A)] + [u(n_9) - u(A)], \\ D_2u &= [u(n_5) - u(A)] + [u(n_8) - u(A)], \end{aligned}$$

Taylor expansions of these finite difference combinations about (x, y) yield

$$\begin{aligned} Tu &\sim \left(\partial_x^2 u + \partial_y^2 u\right) \frac{a^2}{4}, \\ Hu &\sim \left(\partial_x^2 u\right) a^2, \\ D_1u &\sim \left(\frac{1}{4}\,\partial_x^2 u + \frac{\sqrt{3}}{2}\,\partial_x\partial_y u + \frac{3}{4}\,\partial_y^2 u\right) a^2, \\ D_2u &\sim \left(\frac{1}{4}\,\partial_x^2 u - \frac{\sqrt{3}}{2}\,\partial_x\partial_y u + \frac{3}{4}\,\partial_y^2 u\right) a^2, \end{aligned}$$

as $a \to 0$. Now we replace in the motion equations Hu/a^2, $(4T - H)u/a^2$ and $(D_1 - D_2)u/(\sqrt{3}a^2)$ instead of $\partial_x^2 u$, $\partial_y^2 u$ and $\partial_x\partial_y u$, respectively, with similar substitutions for the derivatives of v, thereby obtaining the following equations at each point of the lattice:

$$\begin{aligned} \rho_2 a^2 \frac{\partial^2 u}{\partial t^2} &= 4\mu\, Tu + (\lambda + \mu)\, Hu + \frac{\lambda + \mu}{\sqrt{3}}\,(D_1 - D_2)v, \\ \rho_2 a^2 \frac{\partial^2 v}{\partial t^2} &= 4(\lambda + 2\mu)\, Tv - (\lambda + \mu) Hv + \frac{\lambda + \mu}{\sqrt{3}}\,(D_1 - D_2)u. \end{aligned}$$

The isotropic Navier equations have singular solutions such as

$$\begin{aligned} u &= \frac{a}{2\pi}\left[\tan^{-1}\left(\frac{y}{x}\right)+\frac{xy}{2(1-\nu)(x^2+y^2)}\right], \\ v &= \frac{a}{2\pi}\left[-\frac{1-2\nu}{4(1-\nu)}\,\ln\left(\frac{x^2+y^2}{b^2}\right)+\frac{y^2}{2(1-\nu)(x^2+y^2)}\right], \end{aligned}$$

where $\nu=\lambda/[2(\lambda+\mu)]$ for any a. These solutions represent edge dislocations. We choose (x_0,y_0) different from a lattice point and solve a damped version of the discrete Navier equations

$$\begin{aligned} \rho_2 a^2\frac{\partial^2 u}{\partial t^2}+\gamma\frac{\partial u}{\partial t} &= 4\mu\,Tu+(\lambda+\mu)\,Hu+\frac{\lambda+\mu}{\sqrt{3}}\,(D_1-D_2)v, \\ \rho_2 a^2\frac{\partial^2 v}{\partial t^2}+\gamma\frac{\partial v}{\partial t} &= 4(\lambda+2\mu)\,Tv-(\lambda+\mu)Hv+\frac{\lambda+\mu}{\sqrt{3}}\,(D_1-D_2)u, \end{aligned}$$

with $\gamma>0$. Starting from $(u(x-x_0,y-y_0),v(x-x_0,y-y_0))$, the system relaxes as time grows to a stationary solution that contains a typical heptagon-pentagon defect (sometimes octagons). These are standard defects observed in graphene.

To allow for motion and interaction of these defects taking into account the lattice directions we change coordinates from cartesian coordinates to the primitive lattice coordinates and periodize the differences along them with the lattice constant periodicity [25, 23, 36]. Heptagon-pentagon pairs differently oriented interact through their elastic far fields, attracting and repelling, to form known defects, such as unstable Stone-Wales and different types of dipoles and loops.

4.2 Ripples

The first visualizations of atoms in suspended graphene sheets showed that they were covered with ripples. These ripples are several nanometers long waves of the sheet without a preferred direction. Ripples are expected to be important for electronic transport in graphene, and there is active research about the effects of ripples and strain on electronic properties, including possible strain engineering. These long wrinkles are thermally induced and can be explained by continuum elasticity [41, 42].

In the graphene sheet, carbon atoms have σ bond orbitals constructed from sp^2 hybrid states oriented in the direction of the bond that accommodate three electrons per atom. The other electrons go to p states oriented perpendicularly to the sheet. These orbitals bind covalently with neighboring atoms and form a narrow π band that is half-filled. The presence of bending and ripples in graphene modifies its electronic structure. Out-of-plane convex or concave deformations of the sheet have in principle equal probability and transitions between these deformations are associated with the bending energy of the sheet. A simple way to model this situation to consider that out-of-plane deformations

are described by a double-well site potential that tries to set vertical deflections of the sheet, $w(x,y)$ to $\pm\tilde{w}_0$ and contributes the free energy:

$$F_{DW} = \frac{\tilde{\varphi}}{4}\int \rho_2 \left[1 - \left(\frac{w(x,y)}{\tilde{w}_0}\right)^2\right]^2 dx\, dy,$$

where ρ_2 is the 2D mass density (mass per unit area) and $\tilde{\varphi}$ has units of velocity square. The elastic free energy of the graphene sheet in the continuum limit is that of a 2D membrane,[**?**]

$$F_g = \frac{1}{2}\int [\tilde{\kappa}(\nabla^2 w)^2 + (\tilde{\lambda}u_{ii}^2 + 2\tilde{\mu}u_{ik}^2)]\, dx\, dy,$$
$$u_{ik} = \frac{1}{2}(\partial_{x_k}u_i + \partial_{x_i}u_k + \partial_{x_i}w\partial_{x_k}w),\ i,k = 1,2,$$

where $(u_1,u_2) = (u(x,y),v(x,y))$, $\tilde{\kappa}$, $\tilde{\lambda}$ and $\tilde{\mu}$ are the in-plane displacement vector, the bending stiffness (measured in units of energy) and the 2D Lamé coefficients of graphene (measured in units of force per unit length), respectively. $\nabla = (\partial_x, \partial_y)$ is the 2D gradient and ∇^2 the 2D laplacian. We have ignored the small in-plane nonlinear terms $\partial_{x_i}u\partial_{x_k}u + \partial_{x_i}v\partial_{x_k}v$.

From the total free energy $F = F_g + F_{DW}$, we obtain the equations of motion

$$\begin{aligned}
\rho_2\partial_t^2 u &= \tilde{\lambda}\,\partial_x\left(\partial_x u + \partial_y v + \frac{|\nabla w|^2}{2}\right) + \tilde{\mu}\,\partial_x[2\partial_x u + (\partial_x w)^2] \\
&+ \tilde{\mu}\,\partial_y\left(\partial_y u + \partial_x v + \partial_x w\partial_y w\right), \\
\rho_2\partial_t^2 v &= \tilde{\lambda}\,\partial_y\left(\partial_x u + \partial_y v + \frac{|\nabla w|^2}{2}\right) + \tilde{\mu}\,\partial_y[2\partial_y v + (\partial_y w)^2] \\
&+ \tilde{\mu}\,\partial_x\left(\partial_y u + \partial_x v + \partial_x w\partial_y w\right),
\end{aligned}$$

$$\begin{aligned}
\rho_2\partial_t^2 w = {} & \tilde{P}\nabla^2 w - \tilde{\kappa}\,(\nabla^2)^2 w + \left(1 - \frac{w^2}{\tilde{w}_0^2}\right)\frac{\tilde{\varphi}\rho_2}{\tilde{w}_0^2}w \\
& + \tilde{\lambda}\,\nabla\cdot\left[\left(\partial_x u + \partial_y v + \frac{|\nabla w|^2}{2}\right)\nabla w\right] \\
& + \tilde{\mu}\,\partial_x[2\partial_x u\partial_x w + (\partial_y u + \partial_x v)\partial_y w + |\nabla w|^2\partial_x w] \\
& + \tilde{\mu}\,\partial_y[(\partial_y u + \partial_x v)\partial_x w + 2\partial_y v\partial_y w + |\nabla w|^2\partial_y w] \\
& - (\tilde{\gamma} + \tilde{\eta}w^2)\partial_t w + \sqrt{2\tilde{\theta}(\tilde{\gamma} + \tilde{\eta}w^2)}\,\xi(x,y,t),
\end{aligned}$$

$$\langle\xi(x,y,t)\rangle = 0, \quad \langle\xi(x,y,t)\xi(x,y,t)\rangle = \delta(x-x')\delta(y-y')\delta(t-t'),$$

where $\tilde{P}$ is the membrane stress, $\tilde{\theta}$ is the temperature measured in units of energy and $-(\tilde{\gamma} + \tilde{\eta}w^2)\partial_t w$ is a nonlinear friction force used by Eichler et al to interpret their experiments with a forced damped graphene resonator. The

intensity $\sqrt{2\tilde{\theta}(\tilde{\gamma}+\tilde{\eta}w^2)}$ of the white noise $\xi(t)$ is related to the friction by the fluctuation-dissipation theorem. All the parameters $\tilde{\lambda}$, $\tilde{\mu}$, ρ_2, $\tilde{\kappa}$, $\tilde{P}$, $\tilde{w}_0$, $\tilde{\varphi}$, $\tilde{\gamma}$, $\tilde{\eta}$ and $\tilde{\theta}$ are positive.

The linear operators can then be replaced by periodized elasticity along the primitive lattice direction. Ripples appear that interact con eventual defects [38]. Another possibility consists in representing environmental conditions by means of Glauber spins [41, 37, 33, 34]. Inserting initial conditions corresponding to dislocations loops and dipoles in these models we are able to generate defects with curvature effects and stress fields in accordance with experimental observations [50].

5 Dislocations in crystals

Dislocations are line defects in an elastic crystal [6]. When a sufficiently large stress is applied, these dislocations glide along the crystallographic planes of the crystal and interact with other dislocations they find on their way. In addition, new dislocations are observed to be generated at certain nucleation sites. As a result they appear typically in very large numbers (10^{12} dislocations/cm^2 in heavily worked metals) and modify the mechanical properties of the material. In particular, dislocations are thought to control the plastic properties of crystalline solids (at low temperature).

It is well known that, under an applied stress, crystals deform elastically up to a critical value of this stress, known as the yield stress. For higher stresses, the deformation becomes plastic (irreversible) and ends up eventually in fracture. The yield stress is thought to be the stress at which large numbers of dislocations start moving. Once in the plastic regime, the generation, motion, and interaction of dislocations results in the formation of complicated networks of defects in the microscopic structure of the material. When these networks are so dense that dislocations cannot move freely, the crystal hardens (work hardening). This effect is very important when working with metals, since heavily worked metals are stronger than unworked metals.

Dislocations can be described in many different ways, depending on the lengthscale on which they are viewed. At the microscopic level, they appear as defects in the crystalline lattice. Then, if the separation between dislocations is not too small, there is a mesoscopic scale at which the dislocations may be modelled as line singularities of the elastic stress evolving in a continuous material. Finally, at a macroscopic scale containing large numbers of dislocations we can think in terms of a continuous dislocation density.

5.1 Continuous models for pile-ups

In metal plasticity, we can define an outer length scale as that on which dislocations can be regarded as a line singularity, i.e. the outer equations are the

Navier equations of linear elasticity. The second order strain tensor is defined

$$\boldsymbol{\epsilon} = (\nabla \mathbf{u})^S$$

where $\mathbf{u}$ is the elastic displacement, and the superscript S denotes the 'symmetric part of'. The strain tensor is related to the stress tensor through Hooke's law

$$\boldsymbol{\sigma} = \lambda \mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I} + 2\mu\boldsymbol{\epsilon}$$

where λ and μ are the Lame constants. Finally, the equations of elastic equilibrium are

$$\mathrm{div}(\boldsymbol{\sigma}) = 0.$$

An isolated dislocation can be modelled as a singular solution of these equations in which the displacement is not single valued [1]. This is the classical Volterra model of dislocations. In general, they may be characterized by their tangent vector and a microscopic parameter known as the Burgers vector, which measures the form of the local mismatch in the crystal lattice.

We obtain a model for the interaction of two families of edge dislocations. We take the first family to be tangent to the z-direction and Burgers vector in the x-direction, and the second family to have tangent in the y-direction and Burgers vector in the x-direction. Thus, the first family has the xz-plane as its slip plane, while the second family has the xy-plane as its slip plane, and if we assume that the dislocations remain rectilinear then both families will glide in the x-direction. We refer to them as 'dislocations type 1' and 'dislocations type 2', respectively. By symmetry considerations, the problem can be reduced to a one-dimensional problem [2], giving two populations with densities $w_1(x,t)$ and $w_2(x,t)$, respectively. We want to determine how these density profiles evolve with time.

Conservation of dislocations for both families yields [6]

$$\frac{\partial w_1}{\partial t} + \frac{\partial}{\partial x}(w_1 v_1) = 0,$$
$$\frac{\partial w_2}{\partial t} + \frac{\partial}{\partial x}(w_2 v_2) = 0,$$

where v_i is the velocity of family i. Then, in the absence of any interaction between the families we would close the model with velocity laws such as

$$v_1 = \mathrm{sign}(\sigma_{1,2})|\sigma_{1,2}|^\gamma,$$
$$v_2 = \mathrm{sign}(\sigma_{1,3})|\sigma_{1,3}|^\gamma,$$

In our setting, the first family of dislocations can be seen as a set of lines parallel to the y-axis, and the second family is another set of lines parallel to the z-axis. Both families move along the x-axis. However, as dislocations from the first family move they must cut through the dislocations of the second family. We suppose that there is a strong resistance to this cutting depending on the density

and we consider [2] velocity laws of the form

$$v_1 = \text{sign}(\sigma_{1,2})(|\sigma_{1,2}| - a\sqrt{w_1}),$$
$$v_2 = \text{sign}(\sigma_{1,3})(|\sigma_{1,3}| - a\sqrt{w_2}),$$

with $a > 0$. This is a system of conservation laws that may change type form hyperbolic to elliptic. This corresponds to the onset of pattern formation, formation of dislocation pile-ups. When regularized, we obtain a free-boundary parabolic problem describing the process [6].

5.2 Lattice models for isolated defects

An elementary model for dislocation dynamics in crystal lattices is provided by Frenkel-Kontorova type equations for the displacement $u_n(t)$ of atoms from their equilibrium position along a row in a cubic lattice

$$mu_n'' + \alpha u_n' = d(u_{n+1} - 2u_n + u_{n-1}) - Ag(u_n) + F.$$

All the parameters are positive: m represents the atom mass, α friction, d elastic springs between atoms (interaction strength), F applied force to set the defect in motion. $g(u_n)$ is a periodic function, whose period is given by the lattice constant a. At equilibrium, all atoms are located at lattice positions separated by a distance a in cubic lattices. Dislocations in this framework are represented by a front like solutions, that is, solutions that grow from a stable zero $z_1(F/A)$ of $-Ag(z) + F$ to the next stable zero $z_3(F/A)$, passing through the instable zero $z_2(F/A)$. When $F = 0$, $z_1(F/A) = 0$ and $z_3(F/A) = a$.

If friction is high, the motion is overdamped and we may set $m = 0$ to study it. One can find a threshold $F_c(A)$ such that [3]

- If $|F| \leq F_c(A)$, there are stationary wave front solutions u_n increasing monotonically from $z_1(F/A)$ at $-\infty$ to $z_3(F/A)$ at ∞.
- If $|F| > F_c(A)$ and is close to A, there are traveling wave front solutions $u_n(t) = u(n - ct)$ with wave speed $c(F)$ and profile $u(z)$ solution of

  $$-cu(z) = u(z-1) - 2u(z) + u(z+1) - Ag(u(z)) + F$$

  increasing monotonically from $z_1(F/A)$ at $-\infty$ to $z_3(F/A)$ at ∞. This solution is unique modulo translations.
- traveling and stationary wavefronts cannot coexist.

Stationary wavefronts represent pinned dislocations. Traveling wavefronts represent moving dislocations. $F_c(A)$ represents the Peierls stress needed to move dislocations in the lattice. As $|F| \to F_c(A)$, $c(F) \to 0$, the profiles $u(z)$ develop steps and become discontinuous at $F_c(A)$. This fact is related to a global bifurcation in the system, which is locally of saddle node type and can be used to estimate velocities as $|c(F)| \sim \alpha(F_c)(|F| - F_c(A))^{1/2}$, see [7, 12].

In the absence of friction, or for small friction, we must study the problem with inertia. For piecewise linear g, for instance, $g(u) = u + 1$ if $u < 0$ and $g(u) = u - 1$ if $u > 0$, it is possible to construct explicitly all the branches of traveling wave solutions [14]. In this case, the wave front profiles develop wavy tails. In principle, different wave profiles and speeds are possible. In practice, stability can be proven [15] for a family which displays oscillations only in one tail, the leading edge is monotonic and whose speed surpasses a critical value. We identify two thresholds, the static Peierls stress $F_c(A)$, and the dynamic Peierls stress $F_d(A)$. As before, stationary wavefronts exist when $|F| \leq F_c(A)$. Traveling wavefronts exist when $|F| > F_d(A)$. Both coexist for $F_d(A) < |F| < F_c(A)$. Thus, the system displays hysteresis. As we increase the applied force from zero, wavefront solutions representing dislocations start too move when the force magnitude surpasses $F_c(A)$. Once the dislocation is moving, we can decrease the force below $F_c(A)$, it will still move until it falls below $F_d(A)$. These simulations are done in finite lattices by computational reasons and require nonreflecting boundary conditions, those derived in [32] for instance.

We can study two dimensional dislocations in a cubic lattice by means two dimensional lattice models [11, 13]. In the simplest version, the displacement of the lattice points $u_{i,j}(t)$ in the direction of motion (say, the direction x) is governed by

$$\frac{\partial u_{i,j}}{\partial t} = u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + A(\sin(u_{i,j-1} - u_{i,j})\sin(u_{i,j+1} - u_{i,j})),\ A > 0.$$

Solutions representing dislocations can be generated using elastic far fields of dislocations as initial and boundary conditions [11]. The system relaxes to stationary solutions that represent the corresponding lattice distortion. For instance, if we choose initial and boundary conditions given by $s_{i,j} = \theta(i, j/\sqrt{A}) + Fj$ where θ is the angle function from 0 to 2π and $F > 0$ is a control parameter, we obtain stationary solutions representing edge dislocations for small F. As F grows, stationary solutions will disappear and traveling patterns will be observed [13]. Notice that if we linearize the spatial operator about $s_{i,j}$, we have a discrete elliptic problem for F small but it changes type as F grows.

The idea can be extended to fully 2D and 3D situations by developing 'periodized discrete elasticity lattice models' [17, 20]. We discretize the derivatives appearing the elasticity stress tensor with the required crystal symmetry by means of finite differences in the principal lattice directions, with step equal to the lattice constant, and then periodize, that is, we replace them by periodic functions of the differences, with lattice period. Then, we derive the motion equations with the resulting discrete and periodic stress tensor. For instance, in two dimensions we find

$$\begin{aligned} Mu_1'' = {} & C_{11}D_1^-[g(D_1^+u_1)g'(D_1^+u_1)] + C_{12}D_1^-[g(D_2^+u_2)g'(D_1^+u_1)] \\ & + C_{44}D_2^-[(g(D_2^+u_1) + g(D_1^+u_2))g'(D_2^+u_1)], \\ Mu_2'' = {} & C_{11}D_2^-[g(D_2^+u_2)g'(D_2^+u_2)] + C_{12}D_2^-[g(D_1^+u_1)g'(D_2^+u_2)] \\ & + C_{44}D_1^-[(g(D_1^+u_2) + g(D_2^+u_1))g'(D_1^+u_2)]. \end{aligned}$$

Similar equations are derived for 3D lattices. Dislocation solutions of the corresponding lattices are generated using the known elastic far field for each type of crystal [17, 20].

5.3 Nucleation in lattices

We can use discrete periodized elasticity models to gain insight on the mathematical processes behind defect nucleation. Unlike the models used for large scale molecular dynamics simulations, which implement cut offs to reduce the computational cost, these models involve smooth nonlinearities and are amenable to analysis.

Consider a bidimensional cubic lattice of lattice constant $a = 2\pi$. Let $u_{i,j}(t)$ be the displacement of point (i, j) in the x direction, governed by

$$\begin{aligned} m\frac{\partial^2 u_{i,j}}{\partial t^2} + \alpha\frac{\partial u_{i,j}}{\partial t} &= u_{i-1,j} - 2u_{i,j} + u_{i+1,j} \\ &+A(\sin(u_{i,j-1} - u_{i,j})\sin(u_{i,j+1} - u_{i,j})) \end{aligned}$$

in a square lattice $i = 1, \ldots, N_x$, $j = 1, \ldots, N_y$. We enforce boundary conditions $u_{i,j} = F(j - (N_y + 1)/2)$. This is equivalent to 'shearing' the lattice [21]. As F grows, we observe that the initial zero solution for $F = 0$ changes into slowly varying stationary solutions until we reach a point F_c past which the lattice structure is distorted in two main different ways. Linearizing the problem at $F = F_c$ we find a zero eigenvalue for the resulting matrix, while all the eigenvalues are negative for $F < F_c$. The branch of stationary solutions $s_{i,j}(F)$ is stable. At $F = F_c$ two new branches appear. The system undergoes a pitchfork bifurcation [21].

Changing the geometry we can study other geometries, as for instance, crystal indentation by means of indenters. Now $v_{i,j}(t)$ denotes the vertical displacement, governed by

$$\begin{aligned} m\frac{\partial^2 v_{i,j}}{\partial t^2} + \alpha\frac{\partial v_{i,j}}{\partial t} &= v_{i-1,j} - 2v_{i,j} + v_{i+1,j} \\ &+A(\sin(v_{i,j-1} - v_{i,j})\sin(v_{i,j+1} - v_{i,j})) \end{aligned}$$

in a square lattice $i = 1, \ldots, N_x$, $j = 1, \ldots, N_y$. We set the boundary conditions representing a 'push down' from the central top part:

- Left-hand side: $v_{1,j} = v_{0,j}$.
- Right-hand side: $v_{N_x,j} = v_{N_x+1,j}$.
- Left-hand-side of the top layer ($1 \leq i < p_1$): $v_{i,N_y} = v_{i,N_y+1}$.
- Right-hand-side of the top layer ($p_2 < i \leq N_x$): $v_{i,N_y} = v_{i,N_y+1}$.
- Bottom layer of the domain: $v_{i,0} = 0$.

- Central atoms ($p_1 \leq i \leq p_2$) are pushed downwards according to: $v_{i,N_y+1} - v_{i,N_y} = -f(i)$, where f has a triangular profile, pointing downwards, with magnitude $F > 0$.

As F grows, we observe that the initial zero solution for $F = 0$ develops localized lattice distortions that travel downwards. As we decrease F to zero the distortions travel upwards and may disappear [29]. The branch of stationary solutions that starts at $F = 0$ develops bifurcations at specific values of F at which lattice with different distortions are created. Such new branches are stable for some ranges of F, while the defects simply travel. The configuration bifurcates at new F values, new distortions are created, that travel for while, and the process is repeated as F grows. When we decrease F, the process is reversed. Created distortions travel upwards, and disappear.

6 Bubble and particle formation

6.1 Homogeneous nucleation of particles

Homogeneous nucleation occurs in many examples of first order phase transitions such as condensation of liquid droplets from a supersaturated vapor, glass-to-crystal transformations, crystal nucleation in undercooled liquids, and in polymers, colloidal crystallization, growth of spherical aggregates beyond the critical micelle concentration (CMC), and the segregation by coarsening of binary alloys quenched into the miscibility gap.

Consider a model nucleation in a lattice in which there are many more binding sites, M, than particles, N. We shall consider the thermodynamic limit, $N \to \infty$, with fixed particle density per site, $\rho = N/M$. Let p_k be the number of clusters with k particles or, in short, k clusters, and let $\rho_k = p_k/M$ be the density of k clusters. Particle conservation implies that the total particle density ρ is constant

$$\sum_{k=1}^{\infty} k\rho_k = \rho.$$

In the Becker-Döring kinetic theory of nucleation, a k cluster can grow or decay by capturing or shedding one monomer at a time. Then the evolution with time is given by

$$\rho_k' = j_{k-1} - j_k, \quad k \geqq 2,$$
$$j_k = d_k(e_{(\epsilon_{k+1}-\epsilon_k)/(K_B T)}\rho_1\rho_k - \rho_{k+1}).$$

The monomer density ρ_1 can be obtained from the conservation identity that relates it to the other cluster densities. Different eras in the process of cluster formation can be analyzed by adequate asymptotic methods [16, 18].

6.2 Heterogeneous nucleation

Heterogeneous nucleation happens at preferential sites where irregularities are located.

6.2.1 Bubble formation in radioactive waste

The formation and growth of helium bubbles due to self-irradiation in plutonium has been modeled by discrete kinetic equations for the number densities of bubbles having k atoms. This is an important phenomenon which occurs in radioactive waste and may end up damaging containers resulting in radioactive pollution of the environment. As an alloy ages, there is an initial transient stage during which self-irradiation produces dislocation loops that tend to saturate within approximately two years. The alpha particles created during irradiation become helium atoms. These atoms come to rest at unfilled vacancies generated during their slowing-down process, before they are captured at existing helium bubbles. A helium atom diffuses through the lattice until it finds another helium atom thereby forming a stable dimer or until it finds a helium bubble (a stable cluster with k atoms or, in short, a k-cluster), which absorbes it. Helium bubbles are attached to lattice defects, do not move and do not shed helium atoms because the binding energies of helium to any cluster are extremely high.

We denote by $\rho_k(t)$ the number density of k clusters having effective radii a_k (when the centre of a monomer comes within distance a_k of the cluster centre, it is absorbed). $\rho_1(t)$ is the number of monomers per unit volume, D is the diffusion coefficient and $g(t)$ is the number of monomers created per unit volume and per unit time. The following kinetic model describes the process

$$\begin{aligned} \rho_k' &= 4\pi D\rho_1 a_{k-1}\rho_{k-1} - 4\pi D\rho_1 a_k\rho_k, \quad k \geqq 3, \\ \rho_2' &= 8\pi D\rho_1^2 a_1 - 4\pi D\rho_1 a_2\rho_2, \\ \rho_1 + \sum_{k=2}^{\infty} k\rho_k &= \int_0^t g(s)ds \end{aligned}$$

Asymptotic studies [19] show that this system generates a wave profile describing the evolution of the number of clusters of different sizes with time. A more rigorous analysis is possible after reformulating the system with adequate changes of variables and transforms [35].

6.2.2 Deposition of vapour and particles

Heterogeneous condensation of vapours mixed with a carrier gas in the stagnation point boundary layer flow near a cold wall is considered in the presence of solid particles much larger than the mean free path of vapour particles. The supersaturated vapour condenses on the particles by diffusion, and particles and droplets are thermophoretically attracted to the wall.

Consider a dilute vapour of number density $c(x)$ in a carrier gas that contains a small amount of solid single-size particles. The mass fraction of vapour and of

solid particles are sufficiently small with respect to the mass fraction of the carrier gas, so that the velocity and temperature fields (assumed to be stationary) $u(x)$ and $T(x)$ are not affected by the condensation and deposition processes. The solid particles can act as condensation sites for the vapour. Let n^* be the volume of a particle divided by the molecular volume of condensed vapour, so that a solid particle is equivalent to n^* molecules of vapour. Then a droplet of liquid coating on a solid particle is equivalent to $n(x)$ vapour molecules, in the sense that n equals the volume of a droplet (particle plus condensed vapour) divided by the molecular volume of condensed vapour. Thus, the number of liquid molecules coating a given solid particle is $n(x) - n^*$. Let $\rho(x)$ be the number density of droplets, so that $\rho(x)[n(x) - n^*]$ is the number density of the condensate.

Let us fix a flow geometry, a stagnation point flow near a wall. The equations for $u(x)$, $n(x)$, $T(x)$ and $c(x)$ are [27]

$$
\begin{aligned}
u''' + uu'' + 1 - (u')^2 = 0, \quad x > 0,\\
u(0) = u'(0) = 0,\ u'(\infty) = 1,\\
T'' + Pr\, uT' = 0, \quad x > 0,\\
T(0) = T_w,\ T(\infty) = 1,\\
\left(u + \alpha\frac{T'}{T}\right)\rho' = -\alpha\rho\left(\frac{T'}{T}\right)', \quad x > 0,\\
\rho(\infty) = 1,\\
\left(u + \alpha\frac{T'}{T}\right)n' = -Nn^{1/3}(c - c_e) \quad x_* > x > 0,\\
n(x_*) = 1,\\
c_e(x) = \frac{T_d}{T(x)} exp\left[\frac{1}{\epsilon}\left(\frac{1}{T_d} - \frac{1}{T(x)}\right)\right],\\
c'' + Sc\, uc' = R\rho n^{1/3}(c - c_e), \quad 0 < x < x_*,\\
c(0) = c_e(0),\ c(x_*) = c_e(x_*),\\
c'' + Sc\, uc' = 0, \quad x > x_*,\\
c(x_*) = c_e(x_*),\ c'(x_*^-) = c'(x_*^+)\ c(\infty) = 1,
\end{aligned}
$$

where the point x^* comes with the solution of the free boundary problem [27].

7 Biofilm spread

Biofilms are bacterial aggregates attached to wet surfaces and encased in a self-produced polymeric matrix. This makes them hard to eliminate. At hospitals, they are a major cause of hospital acquired infections. In industry, biofilm induced damage in materials causes substantial losses. On the other side, they are elementary cell aggregates which grow to develop patterns, providing a simple toy system for models of tissue development.

When spreading in flows, biofilms elongate with the current forming threads. The shape of the thread adapts to geometrical constraints, seeking to minimize adequate energies. Its time evolution until an equilibrium shape is reached can be described by discrete rod models. We tackle here two different experimental frameworks: biofilms in networks of cylindrical tubes and biofilms in channel flows. In the latter case, hybrid models combining cellular automata descriptions of cell activity and continuous descriptions of macroscopic fields for chemicals and flows reproduce a rich variety of patterns. Whereas biofilms in flows tend to form filamentary structures, biofilms spreading on agar/air interfaces adopt wrinkled shapes. Hybrid models incorporating elastic fields are also successful reproducing wrinkle formation processes. This section is taken from [43, 48, 51, 52, 54, 57, 58, 64].

7.1 Biofilms in tubes

Consider the typical flow circuits used in medical systems. Injecting bacteria of the *Pseudomonas* genus inside, tubes fill with helical biofilms which wrap around the walls [51]. Vortical motion drive bacteria to the walls creating biofilm nucleation sites. The biofilm then elongates following the streamlines until it undergoes a helical instability.

Discrete rod models describe the process. The filament is discretized using a sequence of nodes $\mathbf{x}^i$ along the filament γ, plus a reference system at each one (the material frame) that measures the twist. This frame is obtained at each location twisting the Bishop frame (a fixed untwisted frame) a certain angle θ^i. The dynamics of the discrete filament is then governed by equations for the angles θ^i, and for the node positions $\mathbf{x}^i$.

The equations for the angles follow from energy arguments. When the undeformed configuration of the filament is straight and its elastic response is isotropic, the elastic energy due to torsion and bending takes the form:

$$E = \sum_{i=1}^{n} \beta \frac{(\theta^i - \theta^{i-1})^2}{\overline{\ell}^i} + \sum_{i=1}^{n} \frac{\alpha}{2\overline{\ell}^i} \sum_{j=i-1}^{i} \|\mathbf{w}_i^j - \overline{\mathbf{w}}_i^j\|^2,$$

where α and β are the bending and torsion moduli, respectively. $\overline{\ell}^i$ is the length of the segments $\overline{\mathbf{e}}^i = \overline{x}^{i+1} - \overline{x}^i$ in a reference undeformed configuration $\{\overline{\mathbf{x}}^0, \overline{\mathbf{x}}^1, ..., \overline{\mathbf{x}}^{n+1}\}$. The vectors $\mathbf{w}_i^j$, $\overline{\mathbf{w}}_i^j$, $j = i-1, i$, are material curvatures in the deformed and undeformed configurations, respectively. The material frame is updated in a quasistatic way. Imposing

$$\frac{\partial E}{\partial \theta^i} = 0,$$

for all segments i not fixed by a boundary condition, this system of equations determines the angle configuration that minimizes the energy of the thread. Clamped ends are accounted for assigning the material frame for $i = 0$, $i = n$. No boundary condition corresponds to a stress free end.

We keep track of the filament position displacing the nodes according to Newton's second law:

$$\mathbf{M}\frac{d^2\mathbf{x}}{dt^2} = -\frac{dE}{d\mathbf{x}} + \mathbf{f},$$

where $\mathbf{f}$ represents the external forces and $-\frac{dE}{d\mathbf{x}}$ the elastic forces. $\mathbf{M}$ is the mass matrix, we set $\mathbf{M} = m\mathbf{I}$. Biofilm filaments live inside tubes of a certain shape. A simple way to incorporate this restriction and reproduce helical instabilities in tubes is a penalty method [51, 57].

7.2 Biofilms in channels

Discrete rod models also allow us to reproduce the dynamics of filaments in corner flows, for instance [57]. The dynamics of biofilm layers covering channel walls, instead, is more appropriately described by means on hybrid models coupling continuous descriptions of flow and chemical fields with cellular automata models of cell activity [43, 52, 58].

Cellular automata provide a simple strategy allowing for an easy transfer of information into macroscopic models. The film is divided in tiles, each of them of the size of a cell. We have to decide for each cell whether it is dead or deactivated, it moves, it detaches or it divides creating a newborn cell that displaces the rest. That is done resorting to probabilities that depend on the relevant concentrations. This approach allows us to use the same grid of tiles to discretize the equations for the concentrations and the displacements.

The fluid surrounding the biofilm is governed by the incompressible Navier-Stokes equations:

$$\begin{aligned} \rho\mathbf{u}_t - \mu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = 0, \qquad & \mathbf{x}\in\Omega_f, t>0 \\ \operatorname{div}\mathbf{u} = 0, \qquad & \mathbf{x}\in\Omega_f, t>0 \end{aligned}$$

where $\mathbf{u}(\mathbf{x},t)$ is the velocity and $p(\mathbf{x},t)$ the pressure. ρ and μ stand for the density and viscosity of the fluid. The non-slip condition on the velocity holds at the biofilm/fluid interface Γ.

Biomass tiles $\mathcal{C}$ located on the surface of the biofilm detach due to shear forces exerted by the flow [52]

$$P_e(\mathcal{C}) = \frac{1}{1+\frac{\gamma}{\tau(\mathcal{C})}} = \frac{\tau(\mathcal{C})}{\tau(\mathcal{C})+\gamma}.$$

γ is a measure of the biofilm cohesion. $\tau(\mathcal{C})$ measures the shear force felt by cell $\mathcal{C}$. The probability for biomass motion in the x directions is defined as:

$$P_x(\mathcal{C}) = \frac{1}{1+\frac{\gamma}{|F_x(\mathcal{C})|}} = \frac{|F_x(\mathcal{C})|}{|F_x(\mathcal{C})|+\gamma}.$$

F_x is the force exerted by the flow in the x direction (on cell walls normal to the x direction) weighted with a geometrical factor accounting for neighbor protection. Similar expressions are used in the y and z directions.

The concentrations of nutrients and oxygen inside the region containing the biofilm and the boundary layer are governed by:

$$c_{s,t} - D_s \Delta^2 c_s = k_2 \frac{c_s}{c_s + K_s} \frac{c_o}{c_o + K_o},$$
$$c_{o,t} - D_o \Delta^2 c_o = \omega k_2 \frac{c_s}{c_s + K_s} \frac{c_o}{c_o + K_o},$$

with zero flux conditions at the substratum. One of them will act as limiting concentration c_l, that is, the concentration that limits biofilm growth. The cells will divide with probability:

$$P_d(\mathcal{C})) = \frac{c_l(\mathcal{C}))}{c_l(\mathcal{C}) + K_l},$$

where c_l denotes the limiting concentration and K_l its saturation coefficient in the Monod law. Whenever neighboring grid tiles are empty, the daughter cell is placed in any of the empty tiles with equal probability. Otherwise, the new cell will shift one of the neighbors. The cell offering the minimal mechanical resistance is chosen [43].

This kind of hybrid models allows us to reproduce a variety of patterns, such as ripples, mounds and streamers, as well as erosion and fragment detachment, on channels of different geometry and roughness [43, 52, 56].

7.3 Biofilms on surfaces

We can reproduce wrinkle branching in an expanding biofilm resorting to Föppl-Von Karman descriptions of the interface biofilm/agar:

$$\begin{aligned}
\frac{\partial \xi}{\partial t} &= \frac{1 - 2\nu_v}{2(1-\nu_v)} \frac{h_v}{\eta_v} \left[D(-\Delta^2 \xi + \Delta C_M) + h \frac{\partial}{\partial x_\beta} \left(\sigma_{\alpha,\beta}(\mathbf{u}) \frac{\partial \xi}{\partial x_\alpha} \right) \right] - \frac{\mu_v}{\eta_v} \xi, \\
\frac{\partial \mathbf{u}}{\partial t} &= \frac{h_v h}{\eta_v} \nabla \cdot \sigma(\mathbf{u}) - \frac{\mu_v}{\eta_v} \mathbf{u},
\end{aligned}$$

where h_v is the thickness of the viscoelastic substratum and μ_v, ν_v, η_v its rubbery modulus, Poisson ratio, and viscosity, respectively. The bending stiffness is $D = \frac{Eh^3}{12(1-\nu^2)}$, where E and ν represent the Young are Poisson moduli of the biofilm, whereas h is the film thickness. ξ stands for the out of plane displacement and $\mathbf{u}$ the in plane displacement. α and β stand for x, y and summation over repeated indices is intended. Stresses σ and strains ε are defined in terms of in-plane displacements $\mathbf{u} = (u_x, u_y)$:

$$\varepsilon_{\alpha,\beta} = \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial \xi}{\partial x_\alpha} \frac{\partial \xi}{\partial x_\beta} \right) + \varepsilon^0_{\alpha,\beta},$$
$$\sigma_{xx} = \frac{E}{1-\nu^2}(\varepsilon_{xx} + \nu \varepsilon_{yy}), \quad \sigma_{xy} = \frac{E}{1+\nu} \varepsilon_{xy}, \quad \sigma_{yy} = \frac{E}{1-\nu^2}(\varepsilon_{yy} + \nu \varepsilon_{xx}).$$

The residual strains $\varepsilon^0_{\alpha,\beta}$ are expressed in terms of the growth tensor as:

$$\varepsilon^0_{\alpha,\beta} = -\frac{1}{2}\left(g_{\alpha\beta} + g_{\beta\alpha} + g_{z\alpha}g_{z\beta}\right),$$

and should be computed from cellular activity.

Using a cellular automata description of cell activity, we can calculate growth tensors due to cell division, death, and water absorption processes, and estimate the residual stresses. Performing ensemble averages, the averaged stresses reproduce spatial variations reflecting cellular activity. Filtering the resulting fields using image processing techniques yields smooth approximations with a clear spatial structure averaging just a few runs. These fields are smooth enough to be plugged in Von Karman's equations without causing numerical instability, allowing to reproduce behaviors that resemble observed patterns [48, 58, 60]. A rigorous existence and stability theory in this type of models is developed in [67, 68].

8 Propagation of electric impulses in semiconductors

Semiconductors are materials of great interest in microelectronics, and are the basis of many devices that exploit the formation of patterns and oscillations in the electric field.

8.1 Discrete models for domain walls in superlattices

Semiconductor superlattices are formed by a sequence of layers of different semiconductor materials. The dynamics of domain walls separating regions with different electric field in semiconductor superlattices is described by systems of the form

$$\frac{dE_i}{dt} + \frac{v(E_i)}{\nu}(E_i - E_{i-1}) - \frac{D(E_i)}{\nu}(E_{i+1} - 2E_i + E_{i-1}) = J - v(E_i),$$

for the electric field E_i at well i. Here, v, D are positive functions and $\nu > 0$ is large. v is a cubic, it grows from 0 to a local maximum, decreases to a positive minimum, and increases to infinity later. For a range of J, we have three zeros $z_1(J) < z_2(J) < z_3(J)$, two of which are stable. For ν large enough, we can construct wavefront solutions [4] and the situation is similar to that described for one dimensional discrete dislocation models. We find thresholds $J_{c_1}(\nu) < J_{c_2}(\nu)$ such that [8]

- If $J_{c_1}(\nu) < J < J_{c_2}(\nu)$, there are stationary wave front solutions E_i increasing monotonically from $z_1(J)$ at $-\infty$ to $z_3(J)$ at ∞.
- If $J_{c_1}(\nu) > J$ or $J > J_{c_2}(\nu)$, there are traveling wave front solutions $E_i(t) = E(i - ct)$ with wave speed $c(J)$ and profile $E(z)$ increasing monotonically from $z_1(J)$ at $-\infty$ to $z_3(J)$ at ∞. Such waves travel with speeds

of opposite sign for each range of J, some of them in the same sense as electrons, some contrary to them.

- traveling and stationary wavefronts cannot coexist.

Stationary wavefronts represent pinned domain walls. Traveling wavefronts represent moving domain walls. As $J \to J_{c_1}(\nu)$ or $J \to J_{c_2}(\nu)$, $c(J) \to 0$, the profiles $E(z)$ develop steps and become discontinuous at the critical values of J. This fact is related to a global bifurcation in the system, which is locally of saddle node type and can be used to estimate velocities as $|c(J)| \sim |\alpha(J_c)|(|J - J_c|)^{1/2}$.

We can add noise $\gamma\xi_i$ to the applied current J, where $\gamma > 0$ characterizes the disorder strength and ξ_i is a zero mean random variable taking values on an interval $(-1, 1)$ with equal probability [10]. Setting $\gamma = 0$, we can repeat with this equation the study done in the previous exercise and obtain a velocity that scales like $|J - J_c|^{1/2}$. However, when we add noise, for each realization of the noise, the thresholds J_c is shifted slightly up or down by the noise. The observed velocity will be the average of the velocities observed for a large number of realizations. For $J > J_c$,

$$|c_R| \sim \frac{1}{\pi}\sqrt{\alpha(J_c)\beta(J_c)(J - J_c) + \gamma\beta(J_c)\xi_0}$$

the average

$$\overline{c} = \frac{1}{N}\sum_{R=1}^{N} |c_R| = \frac{1}{2\pi}\int_{-1}^{1} (\alpha\beta(J - J_c) + \gamma\beta\xi)^{1/2} d\xi \sim (J - J_c^*)^{3/2}$$

where the new critical field is $J_c^* = J_c - \frac{\gamma}{\alpha}$.

As $\nu \to 0$, only fronts traveling in one direction remain, same as for the continuous limit, a reaction-convection-diffusion equation:

$$\frac{dE}{dt} + v(E)E_x - D(E)E_{xx} = J - v(E).$$

8.2 Hyperbolic and kinetic models for the Gunn effect

When we add boundaries and wish to describe the so-called Gunn effect, that is, generation of successive electric pulses at one end which travel and die at the other end, triggering the creation of a new one [5]. This phenomenon is captured at a macroscopic level by the system

$$\begin{aligned}
\frac{\partial^2 E}{\partial x \partial t} + A\frac{\partial E}{\partial t} + B\frac{\partial E}{\partial x} + C\frac{\partial J}{\partial t} + D = 0, &\qquad x \in (0, L),\ t > 0,\\
E(x, 0) = 0, &\qquad x \in (0, L),\\
E(0, t) = \rho J(t), &\qquad t \geqq 0,\\
\int_0^L E(x, t)dx = \phi, &\qquad t \geqq 0,
\end{aligned}$$

where ρ, ϕ, L are positive and A, B, C, D are bounded functions, A and B positive, while C is negative. $E(x,t)$ represents the electric field and $J(t)$ the current, while ϕ is the voltage.

More detailed microscopic models for this phenomena lead to kinetic Boltzmann equations for semiconductors [9, 28] for the carrier density $f(x,k,t)$ such as

$$\partial_t f + \frac{\Delta l}{2\hbar v_M}\sin(k)\partial_x f + \frac{\tau_e}{\eta}F\partial_k f = \frac{1}{\eta}\left[f^{FDa}(k;\mu(n)) - \left(1+\frac{\nu_{imp}}{2\nu_{en}}\right)f + \frac{\nu_{imp}}{2\nu_{en}}f(x,-k,t)\right],$$

$$\partial_x^2 V = \partial_x F = n - 1$$

$$n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x,k,t)\,dk = \frac{1}{2\pi}\int_{-\pi}^{\pi} f^{FDa}(k;\mu(n))\,dk$$

$$f^{FDa}(k;\mu) = \alpha \ln\left[1+\exp\left(\mu - \delta + \delta\cos(k)\right)\right]$$

$$\eta = \frac{v_M}{\nu_{en}x_0} \qquad \delta = \frac{\Delta}{2k_B T}.$$

The boundary conditions are, for $x = 0$:

$$f^+ = \beta F - \frac{f^{(0)}}{\int_0^\pi \sin(k)\, f^{(0)}\,dk}\int_{-\pi}^{0}\sin(k)\, f^-\,dk$$

with

$$\beta = \frac{2\pi\hbar\sigma F_M}{e\Delta N_D}$$

and for $x = L/x_0$:

$$f^- = \frac{f^{(0)}}{(1/(2\pi))\int_{-\pi}^{0} f^{(0)}\,dk}\left(1 - \frac{1}{2\pi}\int_0^\pi f^+\,dk\right)$$

The boundary conditions for the electric potential V are

$$V(0,t) = 0, \quad V(L,t) = \phi_L \sim \frac{\phi}{F_M}\frac{L}{x_0}.$$

The initial condition is

$$f^{(0)}(k;n) = \sum_{j=-\infty}^{\infty}\exp(\imath jk)\,\frac{1-\imath jF/\tau_e}{1+j^2(F)^2}f_j^{FD}(n)$$

$$f_j^{FD}(n) = \frac{1}{\pi}\int_0^\pi f^{FD}(k;\mu(n))\,\cos(jk)\,dk$$

with $x \in [0, L = L/x_0]$ and f periodic in k with period 2π. The average energy E is defined as

$$E = \frac{E}{k_B T} = \frac{\int_{-\pi/l}^{\pi/l} \varepsilon(k) f(x,k,t)\, dk}{k_B T \int_{-\pi/l}^{\pi/l} f(x,k,t)\, dk} = \delta \frac{\int_{-\pi}^{\pi} (1-\cos k)\, f(x,k,t)\, dk}{\int_{-\pi}^{\pi} f(x,k,t)\, dk}.$$

This model implements a BGK approximation of the collision kernel in the equation for the carrier density. The full model involves a nonlocal collision kernel and equations for different types of carriers [9].

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