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# Mathematics of Computational Modelling: some challenges of computing nonlinear phenomena

**Abstract:** The prediction of various phenomena through models and computation is a necessity in numerous real life problems. The computation of singular phenomena (interfaces, shocks, defects, cracks...) arises in many complex systems and poses many challenges. For computing such phenomena, it is natural to seek methods that are able to detect them and to devote the necessary computational recourses to their accurate resolution. These phenomena are very interesting for their importance and applicability, but also for the challenge they pose in mathematical research. From a computational perspective we need to design algorithms that are fast but also reliable. In this paper we consider examples of such phenomena modelled by nonlinear Partial Differential Equations and discrete microscopic systems. Since often weak solutions of PDEs related to these problems are not unique, we demonstrate that "natural ad hoc" computational methods might predict irrelevant solutions. Since numerical methods perturb the mathematical model, mathematical analysis emerges as a necessary tool which ensures that our computational methods approximate physically relevant solutions. We discuss in more detail three nonlinear problems: (i) A problem related to design and analysis of approximate atomistic-continuum energies to atomistic models arising in crystalline materials (ii) A problem of cell interaction within a fibrin medium. Motivated by experiments we demonstrate that the combination of sophisticated mathematical modelling and numerical analysis leads to reliable computational predictions and reveals the real mechanisms of the observed interactions (iii) A problem arising in statistical inference of solutions to nonlinear hyperbolic systems. To compute measure valued solutions, we propose new discrete kinetic models and we study corresponding kinetic formulations of viscus and inviscid conservation laws.

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# 1 Introduction

Numerical Analysis and Scientific Computing, i.e., the Mathematics and Algorithms of approximations, have been one of the most rapidly developing fields during the era of the technological innovation. Novel mathematical methods and computational techniques have set new standards in engineering and scientific computing by solving problems that were beyond reach some years ago and by providing new challenges for technological innovation. This progress goes hand in hand with the development of the other two pillars of Applied Mathematics: Modeling and Analysis.

Most of the mathematical models describing nonlinear phenomena exhibit complicated structures, and their study poses serious challenges for mathematical research. Often these models describe singular phenomena (interfaces, shocks, defects, dislocations, ...). Their understanding is quite involved and important since they arise in many diverse applications. The computation of such structures poses an enormous challenge for applied mathematicians and engineers. Starting from the work of J. von Neumann, the non expected behaviour of standard numerical schemes intrigued mathematicians and scientists, leading to fundamental developments in several areas of mathematics and engineering. A key element, which distinguishes the computation of nonlinear phenomena to other more traditional problems, is their sensitivity to small perturbations. Thus, seemingly controllable errors might change completely the character of the computed solution leading to "physically" irrelevant predictions. As it is natural, this procedure can have catastrophic effects in algorithm design. All numerical procedures generate errors, and thus the schemes induce their own physics into the problem. A careful and systematic analysis, based in most of the cases on deep mathematical methods, is required in order to provide some guarantees that we indeed compute physically relevant approximations. Given that non-trivial nonlinear phenomena appear in many diverse applied problems, mathematics of computational modelling appears a necessity for reliable predictions.

In Section 2 we discuss issues related to the sensitivity of schemes in computing nonlinear phenomena. Next we describe in more detail three nonlinear problems: In Section 3, a problem related to design and analysis of approximate atomistic-continuum energies to atomistic models arising in crystalline materials. In Section 4, a problem of cell interaction within a fibrin medium. Motivated by experiments we demonstrate that the combination of sophisticated mathematical modelling and numerical analysis leads to reliable computational predictions and reveals the real mechanisms of the observed interactions. In Section 5, a problem arising in statistical inference of solutions to nonlinear hyperbolic systems. To compute measure valued solutions, we propose new discrete kinetic models and we study corresponding kinetic formulations of viscus and inviscid conservation laws.

# 2 Sensitivity of schemes

We are interested in approximating mathematical models described by differential equations. Our aim is to design schemes which lead to *fast and reliable algorithms*. Typically error estimates of a priori or a posteriori type provide mathematical guarantees including among others the convergence to the exact solution. Quite often, the correct asymptotic behaviour is not sufficient, and we need to test our approximating methods against other criteria. A key issue emerges when we require for our schemes to *preserve key structural properties of the problem*. In particular, for non-linear phenomena, this property is quite important, and one of the key elements in scheme design. Preserving structural properties is not trivial as the following elementary example shows: Let $A \in \mathbb{R}^{m,m}$ be an *antisymmetric* matrix, $A^T = -A$. Consider the initial value problem

$$y'(t) = Ay(t), \quad t \geq 0, \qquad y(0) = y_0.$$

Then the norm $\|y(\cdot)\|$ is constant in time, $\|y(t)\| = \|y(0)\|$. This property at certain more involved applications is related to "energy conservation." We would like to preserve this property at the computational level. However, although both Backward Euler, $y^{n+1} - y^n = hAy^{n+1}$, and Trapezoidal Methods, $y^{n+1} - y^n = \frac{h}{2}Ay^{n+1} + \frac{h}{2}Ay^n$, are natural approximating schemes, only the second one satisfies the discrete analog of the energy conservation, as a simple calculation shows. More generally, one can observe that preserving structural properties often serves as a useful design principle of the computational algorithm.

*Nonlinear problems with non unique weak solutions.* Consider the nonlinear evolution PDE written in abstract form

$$u_t(t) + A(u(t)) = 0.$$

This is a nonlinear evolution PDE such as, e.g., Conservation Laws (CL), Hamilton Jacobi equations (HJ) and equations describing phase separation. For several such problems one is interested in solutions with reduced smoothness. Such *weak solutions* are appropriately defined and there is a rich mathematical theory related to their study. Often, such solutions are not unique and one has to impose additional selection criteria which hopefully pick the *physical relevant* solution (CL: entropy solution, HJ: viscosity solution, geometric laws for propagating interfaces). As far as the mathematical justification is concerned, nonlinear PDE theory provides partial answers - (CL: Kruzkov's theory for the scalar case, HJ: theory of viscosity solutions of Crandall-Lions, measure valued solutions ....) Although complete theories are available for a limited number of interesting problems, these theories provide important insight and highlight subtle points in the design of physically relevant schemes. As we shall see, the design of appropriate

computational schemes for such problems is quite delicate. One of the main obstacles one has to overcome is the possibility the numerical method to pick at the limit a weak solution which is not however the physically relevant one. A way out is the careful design based on preserving structural properties at the discrete level.

*A typical example: Scalar Conservation Laws.* Consider the nonlinear equation

$$u_t(x,t) + \mathrm{div}F(u(x,t)) = 0, \quad x \in \mathbb{R}^d, t > 0. \tag{2.1}$$

Weak solutions are defined through a variational formulation and admit solutions which are even discontinuous. Among them uniqueness is guaranteed by imposing an infinite number of additional variational inequalities: The unique *entropy* solution satisfies

$$\eta(u)_t + \mathrm{div}Q(u) \leq 0, \quad \text{in } \mathcal{D}'.$$

Here, $\eta$ is convex and $\eta, Q$ an entropy entropy-flux pair, [16]. An alternative characterisation of the entropy solution emerges as the limit of viscosity approximations ("viscosity solution") $u^\epsilon \to u$ where

$$u_t^\epsilon(x,t) + \mathrm{div}F(u^\epsilon(x,t)) = \epsilon\Delta u^\epsilon(x,t), \quad x \in \mathbb{R}^d, t > 0. \tag{2.2}$$

This interpretation of the entropy solution has subtle consequences in the scheme design. Firstly, it hints that successful approximations should include a form of *artificial diffusion,* [60]. On the other hand, since not all perturbations of (2.1) lead to the entropy solution, one should be rather sure that the scheme does not implicitly induce unwanted perturbations, since, in general, different regularisations might pick different solutions at the limit. In fact, *"reasonable"* schemes do not perform always as we expect. The main reason is that each scheme approximating (2.1) is modelled by a PDE of the form

$$v_t^h(t) + \mathrm{div}F(v^h(t)) = B_h(h, v^h(t)),$$

where $B_h(h, v^h(t))$ is a differential operator acting on $v^h$ which is not always easy to write explicitely. To fix ideas, consider the one dimensional conservation law

$$u_t + F(u)_x = 0.$$

A quite natural discretisation scheme is the "central scheme" (discretisation in $x$ only)

$$\frac{d}{dt}u_i(t) = -\frac{1}{2h}(g_{i+\frac{1}{2}} - g_{i-\frac{1}{2}}) = -\frac{F(u_{i+1}) - F(u_{i-1})}{2h}.$$

This scheme is a second order approximation of the conservation law and third order approximation of

$$u_t^h + F(u^h)_x = \alpha h^2 F(u^h)_{xxx}.$$

Thus explaining the oscillatory behaviour, due to dispersive perturbation, see Fig 1. For the very interesting limit dynamics of such schemes and dispersive perturbations,

see [59, 33]. In Hou and Lax [33] a very interesting historical account regarding the pioneering contributions of J. von Neumann to the birth of computational fluid dynamics is included. For related works regarding the development of the mathematical theory of small dispersion limits, see [36, 58, 37]. In Fig. 2 one can find another example of scheme sensitivity in computational fluid dynamics, [6], where the discrete divergence free condition in finite element Navier-Stokes solvers is destroyed due to mesh refinement.
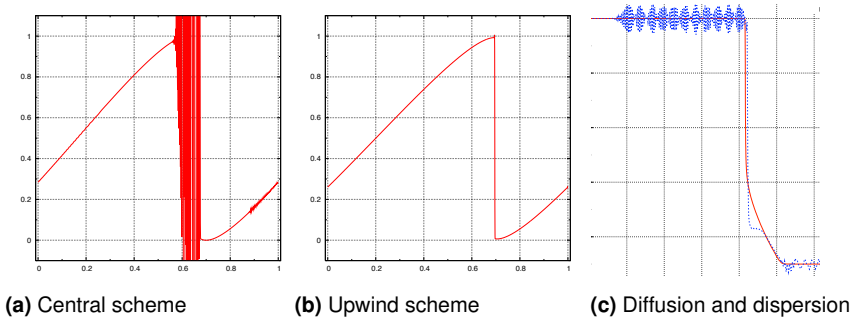


**(a)** Central scheme   **(b)** Upwind scheme   **(c)** Diffusion and dispersion

**Fig. 1:** An oscillatory central scheme (A) and a shock capturing upwind scheme (B) for Burgers equation. Two schemes approximating different weak solutions in the case of non-convex flux function (C).
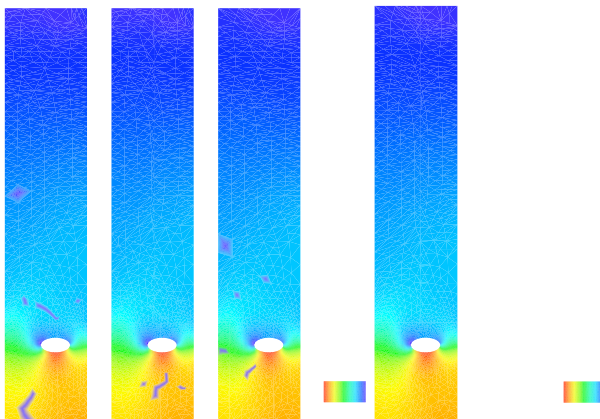


**Fig. 2:** Severe pressure pollution in Navier-Stokes solvers: von Karman vortex shedding with random mesh refinement at several places. Pressure jumps at places where you refine.

*Numerical issues on PDE/multiscale Energy Minimisation.* Another important class of *nonlinear problems with non unique weak solutions* are arising in minimisation problems. Issues, such as computation of phase transitions and other singular or nearly singular phenomena appear here as well. The mathematics of these quite diverse problems are very rich, but still, provide understanding only in limiting cases, [4]. From the computational perspective, although numerical optimisation is quite advanced, the numerical analysis of PDE and multi-scale energy minimisation is not quite developed and many questions and problems remain unexplored. Consider the nonlinear minimization problem

find a local minimizer $v$ in $\mathcal{V}$ of :

$$\mathcal{E}(v)\,,$$

where usually $\mathcal{E}$ is in general non-convex, $\mathcal{E}$ has more than one critical points and $\mathcal{E}$ is often singularly perturbed (including regularisation terms). In atomistic models $\mathcal{E}$ is discrete but includes long range interactions and minimizers depend on the space $\mathcal{V}$ and its properties. The approximate energy minimisation problem is posed over finite dimensional spaces $V_h$, and approximating energy functionals $\mathcal{E}_h$ :

find a local minimizer $v$ in $\mathcal{V}_h$ of :

$$\mathcal{E}_h(v)\,.$$

Many questions arise, since for example the relationship between $\mathcal{E}_h$ and $\mathcal{E}$ might not be always clear. In particular, questions such as what are the appropriate choices of the approximate energies $\mathcal{E}_h$ emerge in several applications. Similarly, the relationship between $\mathcal{V}_h$ and $\mathcal{V}$ is quite subtle, as for example it might fall into unrealistic approximate minimisers due to Lavrentiev phenomenon, see Ball and Knowles, [5]. An indicative example reflecting the sensitivity of discretisation methods, and the very different nature of the resulting approximations is provided by the next simple scalar problem of phase separation. The energy functional is

$$\mathcal{E}_\varepsilon(u) = \int_\Omega \left[ \varepsilon\, |\nabla u|^2 + \frac{1}{\varepsilon}(u^2 - 1)^2 \right] dx\,.$$

When the domain $\Omega$ is convex the minimisers are two constant states $u = 1$ or $u = -1$. In the case of non-convex $\Omega$, several interesting solutions emerge, e.g., [35]. However, even in the simplest case the computation of minimisers is far from straightforward. Unphysical interfaces emerge, and the computational solutions are quite sensitive on mesh discretisation parameters, see Figure 3.
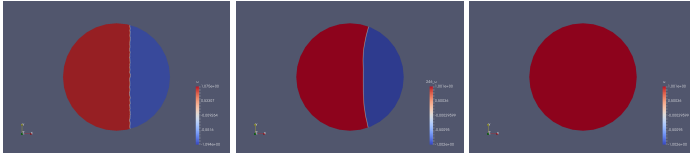
**Fig. 3:** Three entirely different approximate solutions with mesh resolution $h$, $h/2.9$, and $h/3.3$ respectively.

# 3 Consistent atomistic-continuum energies

Most real world systems include a description at several scales, i.e., they are multi-scale in nature. Our understanding in models from physics is by far the best, however, even there, many issues remain mathematically unexplored or inaccessible by computational means. In several complex applications involving multiple scales, notably in materials science and nanotechnology, the closure laws are either not known, or hold in restrictive situations. Even when effective laws are known, understanding the underlying mechanisms and the rigorous passage across scales up to the continuum level (quantum, atomistic, kinetic, continuum) constitutes a key challenge in applied mathematics. From a computational prespective, the huge number of degrees of freedom of the microscopic problems, as well as, the possible singular behaviour of the underlying phenomena constitute the main bottleneck for important developments. Usually, effective theories fail when singular phenomena appear, e.g., the passage from atomistic to continuum is typically valid only when certain smoothness criteria are met. A way to overcome this problem at a computational level is to use hybrid models across scales, i.e., to use different models in different areas of the computational domain. We would like to study models where the microscopic model is kept in the areas of singular behaviour and macroscopic models are used in the areas of smoothness. Numerical Analysis motivates the design of new consistent models which accurately link the two scales of the problem. In this section we will see how one can address this problem when coupling between atomistic and continuum descriptions is chosen.

*Atomistic Models* . We consider a simple scaled two dimensional lattice $\varepsilon \mathbb{Z}^2 = \{x_\ell = (x_{\ell_1}, \ldots, x_{\ell_d}) = \varepsilon \ell, \ell \in \mathbb{Z}^2\}$. We shall assume that atoms are placed initially at the lattice points $x_\ell$ and the interatomic distance is $\varepsilon$ . Without being very precise about the notational conventions we will consider discrete periodic functions on $\mathbb{Z}^2$ defined over a 'periodic domain' $\mathcal{L}$ and $\Omega_{\text{discr}} := \varepsilon \mathbb{Z}^2 \cap \Omega, \quad \mathcal{L} := \mathbb{Z}^2 \cap \frac{1}{\varepsilon} \Omega$. We consider atomistic
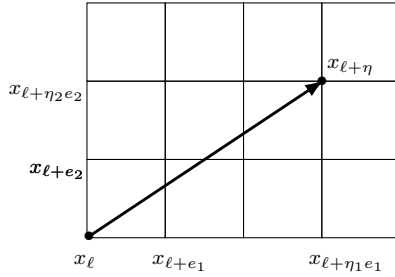
**Fig. 4:** Two dimensional lattice.

deformations

$$y_\ell = y(x_\ell), \quad \ell \in \mathcal{L} \quad \text{of the form}$$

$$y_\ell = Fx_\ell + v_\ell, \quad \text{with } v_\ell = v(x_\ell) \text{ periodic with respect to } \mathcal{L}.$$

The corresponding spaces for $y$ and $v$ are denoted by $\mathcal{X}$ and $\mathcal{V}$ :

$$\mathcal{X} = \{y : \mathcal{L} \to \mathbb{R}^2, \quad y_\ell = Fx_\ell + v_\ell, \quad v \in \mathcal{V}\},$$

$$\mathcal{V} = \{u : \mathcal{L} \to \mathbb{R}^2, \quad u_\ell = u(x_\ell) \quad \text{periodic with respect to } \mathcal{L}\}.$$

For functions $y, v \; : \; \mathcal{L} \to \mathbb{R}^2$ we define the product $\langle y, v \rangle_\varepsilon := \varepsilon^2 \sum_{\ell \in \mathcal{L}} y_\ell v_\ell$. The energy of a deformed crystal is described through given potentials accounting for interactions between atoms. We consider the atomistic potential

$$\Phi^a(y) = \varepsilon^2 \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta (\overline{D}_\eta y_\ell),$$

where $R$ is the set of interaction vectors. and

$$\overline{D}_\eta y_\ell = \frac{y_{\ell+\eta} - y_\ell}{\varepsilon}, \qquad \ell, \ell + \eta \in \mathcal{L}.$$

Notice that the atomistic potential is a highly nonlinear function involving "discrete derivatives". For a given field of external forces $f : \mathcal{L} \to \mathbb{R}^2$ the *atomistic problem* reads:

find a local minimizer $y^a$ in $\mathcal{X}$ of :

$$\Phi^a(y^a) - \langle f, y^a \rangle_\varepsilon.$$

Notice that as the atomistic problem is a discrete energy minimization problem, its Euler-Lagrange equations will give rise to a "nonlinear finite difference" system. In fact, if such a minimizer exists, then

$$\langle D\Phi^a(y^a), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon, \qquad \text{for all } v \in \mathcal{V}.$$

Here,

$$\langle D\Phi^a(y), v\rangle_\varepsilon = \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \nabla_\zeta \phi_\eta \left(\overline{D}_\eta y_\ell\right) \cdot \overline{D}_\eta v_\ell.$$
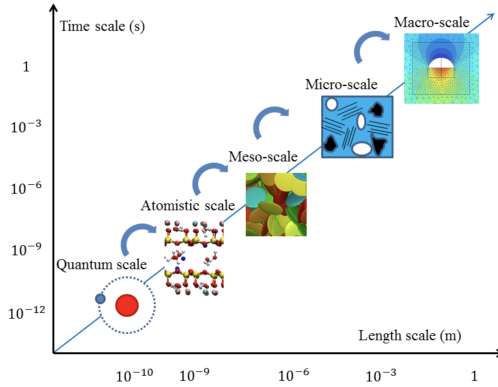


**Fig. 5:** Macro-scale : continuum models – Partial Differential Equations, Meso-scopic models: Kinetic models, Meso-scopic models : coarse grained atomistic models.

*A continuum model for smooth deformations: the Cauchy-Born approximation.* One would like to approximate the atomistic model by a continuum energy minimisation problem. Notice that we adopt a reverse point of view compared to the standard one in numerical analysis for PDEs, in the sense that the atomistic problem is the exact problem (discrete difference scheme) and we aim to find a continuum approximation (a PDE) to the atomistic model. This is not a trivial task, and in fact, such approximations are meaningful only when smooth deformations are considered. When smoothness is lost, e.g., when defects or cracks appear, the continuum modelling becomes quite subtle and various approaches proposed so far are still under debate. Notice, however, that we intend to use the continuum model only locally at smooth areas. To this end, we define the Cauchy-Born stored energy function, [24], as

$$W(F) = W_{CB}(F) = \sum_{\eta \in R} \phi_\eta \left(F \eta\right).$$

The Cauchy-Born energy minimisation problem is

find a local minimizer $y^{CB}$ in $X$ of :

$$\Phi^{CB}(y) - \langle f, y^{CB}\rangle = \int_\Omega W(\nabla y^{CB}) - \langle f, y^{CB}\rangle.$$

Here

$$X = \{y : \Omega \to \mathbf{R}^d, \quad y(x) = Fx + v(x), \ v \in V\},$$

$$V = \{u : \Omega \to \mathbf{R}^d, \quad u \in W^{k,p}(\Omega, \mathbf{R}^d) \cap W^{1,p}_{\#}(\Omega, \mathbf{R}^d), \int_\Omega u dx = 0\}.$$

The Euler-Lagrange equations are a system of nonlinear PDEs:

$$\langle D\Phi^{CB}(y), v \rangle = \int_\Omega S_{i\alpha}(\nabla y(x)) \, \partial_\alpha v^i(x) \, dx = \langle f, v \rangle, \qquad v \in V,$$

where the stress tensor is defined as $S := \left\{ \frac{\partial W(F)}{\partial F_{i\alpha}} \right\}_{i\alpha}$. Some remarks on the relation between the atomistic and continuum CB models are in order. As mentioned, the continuum model approximates the atomistic model only when deformations are sufficiently smooth, however, the mathematical justification of this approximation is far from straightforward. Key technical difficulty is due to the fact that the interatomic potentials allow for long range interactions as opposed to interactions only of next neighbours (only adjacent atoms interact). The main results based on different notions of consistency (the term is borrowed from standard numerical analysis terminology) start with the *Variational Consistency:*

$$\mathcal{C}_V(y) := \sup \Big\{ \, |\langle D\Phi^a(y), v \rangle_\varepsilon - \langle D\Phi^{CB}(y), v \rangle| \, :$$

$$v \in \mathcal{V} \quad \text{with } \|v\|_{W^{1,p}(\Omega)} = 1 \, \Big\},$$

where in the last relation $y$ is any smooth function. We shall refer to $\mathcal{C}_V(y)$ as the *variational consistency error*. Similarly we define the *Energy Consistency error* by

$$\mathcal{C}_\mathcal{E}(y) := |\Phi^a(y) - \Phi^{CB}(y)|.$$

We aim to estimate both $\mathcal{C}_V(y)$ and $\mathcal{C}_\mathcal{E}(y)$ in terms of powers of $\varepsilon$, yielding two consistency criteria, one for the energies and one for the first variations. Consistency errors account, as in Numerical Analysis, to the extent to which an exact smooth solution fails to satisfy the approximating scheme. Given that the stability of the scheme is satisfactory, usually the consistency error determines the order and therefore the quality of the approximation. This includes the case where consistency errors do not tend to zero as the mesh parameter (here represented by the the interatomic distance $\varepsilon$) does. In this case it is well known that convergence is lost.

**Theorem 3.1** (Energy consistency). *Let $y$ be a smooth function. Then the atomistic energy $\Phi^a(y)$ is a second order approximation of the continuum Cauchy-Born energy $\Phi^{CB}(y)$ in the sense that there exists a constant $M_E = M_E(y)$,*

$$\left| \Phi^a(y) - \Phi^{CB}(y) \right| \leq M_E \, \varepsilon^2.$$

The above result was obtained by Blanc, LeBris & Lions, [9]; a similar problem in the case where we include surface energies was addressed in [53]. We have a similar bound for the first variations given in the following theorem.

**Theorem 3.2** (Variational consistency). *Let $y$ be a smooth function; then, for any $v \in \mathbb{V}_h$, the continuum Cauchy–Born variation $\langle D\Phi^{CB}(y), v \rangle$ is a second-order approximation to the atomistic variation $\langle D\Phi^a(y), v \rangle_\varepsilon$ in the sense that there exists a constant $M_V = M_V(y, p)$, $1 \le p \le \infty$, independent of $v$, such that*

$$\left| \langle D\Phi^{CB}(y), v \rangle - \langle D\Phi^a(y), v \rangle_\varepsilon \right| \le M_V \, \varepsilon^2 \, |v|_{W^{1,p}(\Omega)}.$$

This result was first stated by E. & Ming, [23]. The first systematic proof was given in [46] by introducing a new finite element consistency analysis appropriate for atomistic problems, see also [48] for an alternative approach.

*Coupled Atomistic-Continuum methods.* The idea of coupling energies, pioneered in, e.g., [56, 13], is at the heart of designing principles of the *multiscale methods,* i.e., of computational methods which are able to tackle models at different scales simultaneously. However, initial attempts to couple the local energies, led to artefacts and computational inconsistencies. The important unresolved issue is the mechanism for coupling the atomistic and the continuum model, specifically, the "interface conditions" needed for the exchange of information between the two scales. Since the atomistic models involve long range interactions, and thus nonlocal effects, this is a highly non-trivial task. The term "ghost-forces" was used —initially in the engineering literature— for the unphysical behaviour observed on the interface of these two regions. This is essentially a manifestation of the loss of consistency for the first variations, i.e., coupled energies had $\mathcal{C}_V(y) = O(1)$ while $\mathcal{C}_E(y)$ was at least $O(\varepsilon)$ (with the obvious modifications in the definitions).

Thus the following consistency criterion seemed important: the energy $\mathcal{E}$ is said to be *free of ghost forces* if

$$\langle D\mathcal{E}(y_F), v \rangle = 0, \quad y_F(x) = Fx, \tag{3.1}$$

for all appropriate variations $v : \bar{\Omega} \cap L \to \mathbb{R}^2$ such that $v_\ell = 0$ outside a compact set. This requirement has more than one interpretation. Firstly, it is clear that affine deformations are energy minimisers for both the atomistic and the Cauchy-Born model, and thus it is quite natural to require that the same property is preserved for coupling energies. The requirement (3.1) is related to variational consistency. The analysis in [34] shows that when (3.1) fails, $\mathcal{C}_V(y) = O(1)$, and vice-versa. When we design a method aiming at optimising the rate of $\mathcal{C}_V(y)$, the coupled energies satisfy (3.1). We claim that, as it is the case for all important structural properties, it is not a good idea to ignore this
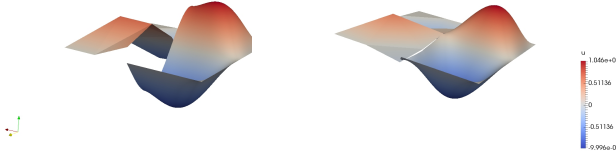
**Fig. 6:** Ghost forces for the Laplace equation, the domain is divided in two, using fine mesh in $\Omega_1$ and coarse mesh in $\Omega_2$.: inconsistent coupling (left) and consistent coupling (right). The two solutions differ more than 20% even away from the interface, [45].

requirement at the design level. Variational inconsistency for coupled energies might have catastrophic effects even for linear problems as the example in Fig. 6 highlights. Next we describe the *design principles of coupling methods* which will satisfy (3.1). We define $\Omega_a$ as the atomistic region, $\Omega_*$ as the atomistic Cauchy-Born region and $\Gamma$ as the interface between $\Omega_a$ and $\Omega_*$ which has no thickness. Also, $\Omega$ is the whole region being examined which contains $\Omega_a$, $\Omega_*$ and $\Gamma$ such that

$$\bar{\Omega} = \bar{\Omega}_a \cup \bar{\Omega}_*, \quad \Gamma = \bar{\Omega}_a \cap \bar{\Omega}_*.$$

For a fixed $\eta \in R$, a bond can be defined as the line segment $b_\ell = \{x \in \mathbb{R}^2 : x = \ell + t\eta, \ 0 < t < 1\}$. A *bond volume* $B_{\ell,\eta}$ that corresponds to $b_\ell$ is the interior part of a parallelogram that has a diagonal $b_\ell$, i.e.,

$B_{\ell,\eta}$ is an open quadrilateral that has vertices $x_\ell, x_{\ell+\eta_1 e_1}, x_{\ell+\eta_2 e_2}, x_{\ell+\eta}$ .

The following lemma is quite useful.

**Lemma 3.3.** *Let $v \in \mathbb{Q}_1(B_{\ell,\eta})$, then*

$$\varepsilon^2 \overline{D}_\eta v_\ell = \frac{1}{\eta_1 \eta_2} \int_{B_{\ell,\eta}} \nabla v(x)\eta \, dx .$$

We highlight how the *discontinuous coupled method* can be designed. The method, introduced in [43], allows flexibility on the construction of the underlying meshes and the computation of the energy at the interface is not involved. To retain consistency the interfacial energies should include terms accounting for the possible discontinuity of the underlying functions, and hence the name discontinuous coupling.

The design of the method is done with respect to the bond volumes $B_{\ell,\eta}$. Specifically, we consider three cases which are determined by the location of bond volume $B_{\ell,\eta}$ with respect to the interface: (a) $\overline{B}_{\ell,\eta} \subset \Omega_a$: The closure of bond volume $\overline{B}_{\ell,\eta}$

is contained in $\Omega_a$, in this case the atomistic energy is used. (b) $B_{\ell,\eta} \subset \Omega_*$: The bond volume $\overline{B}_{\ell,\eta}$ is contained in region $\Omega_*$, in this case the continuum energy is used. (c) $B_{\ell,\eta} \in B_\Gamma$ if it intersects the interface, i.e $\overline{B}_{\ell,\eta} \cap \Gamma \neq \emptyset$. In the last case we need to design new energies which will account for seamless communication between the two different models. To this end, the contribution to the energy which corresponds to (a), for a fixed $\eta$, is:

$$E^a_{\Omega_a,\eta}\{y\} = \varepsilon^2 \sum_{\substack{\ell \in \mathcal{L} \\ \overline{B}_{\ell,\eta} \subset \Omega_a}} \phi_\eta(\overline{D}_\eta y_\ell).$$

For a fixed $\eta$, the contribution to the energy which corresponds to the CB region is

$$E^{a,cb}_{\Omega_*,\eta}\{y\} = \int_{\Omega_*} \phi_\eta(\overline{\nabla} y(x)\eta)dx$$

where for technical reasons we consider $\overline{y}$ to be the piecewise bilinear function at the lattice cells, for the general finite element decomposition of the continuum region see [43]. Without being very specific, to define the interface energy we need to consider piecewise polynomial functions $y^{\ell,\eta}$ defined on $B_{\ell,\eta}$ as follows: $\overline{y}^{\ell,\eta} \in \mathbb{Q}_1(K)$ interpolating $\{y_\ell\}$ for all atomistic cells $K \subset \Omega_*$. In the remaining part of the bond volume (contained in $\Omega_a$), $y^{\ell,\eta}$ is defined by interpolating lattice values, see [43, 34]. Then it follows that this function is continuous on $B_{\ell,\eta} \backslash \Gamma$ and possibly discontinuous on the interface $\Gamma$. Our work identifies this discontinuity as the source for the loss of the variational consistency. Based on these observations, the energy for the bond volumes intersecting the interface can be defined as

$$E^D_{\Gamma,\eta}\{y\} = \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,\eta} \in B_\Gamma}} \frac{1}{|\eta_1\eta_2|} \Big[ \int_{B_{\ell,\eta}} \chi_{\Omega_a} \phi_\eta(\nabla y^{\ell,\eta}\eta) \, dx$$

$$- \int_{B_{\ell,\eta} \cap \Gamma} \nabla_\zeta \phi(\{\!\{\nabla y^{\ell,\eta}\eta\}\!\}) \cdot [\![y^{\ell,\eta}\eta]\!] \, dS \Big]. \qquad (3.2)$$

Here, $[\![w\eta]\!]$ denotes the jump and $\{\!\{w\}\!\}$ denotes the average of a possibly discontinuous function on the interface

$$[\![w\eta]\!] := (\nu_{\Omega_a} \cdot \eta) \, w^- + (\nu_{\Omega_*} \cdot \eta) \, w^+, \qquad \{\!\{w\}\!\} := \frac{1}{2}\{w^- + w^+\}, \qquad (3.3)$$

where $w^-$ is the limit taken from $\Omega_a$ and $w^+$ is the limit taken from $\Omega_*$. Also, $\nu_{\Omega_a}$ and $\nu_{\Omega_*}$ are the respective exterior normal unit vectors, that satisfy $\nu_{\Omega_a} = -\nu_{\Omega_*}$ on $\Gamma$. The last term in (3.2) is added to account for the loss of continuity of the underlying functions and its choice is related to the design of Discontinuous Galerkin finite element methods, see the next section for related problems at the continuum level. For such

methods, it is essential to add penalty terms for stability reasons. Finally, for a penalty parameter coefficient $\gamma_P > 0$ the interfacial energy takes the form,

$$\tilde{E}^D_{\Gamma,\eta}\{y\} = E^D_{\Gamma,\eta}\{y\} + \frac{\gamma_P}{\varepsilon} \sum_{\substack{\ell \in \mathcal{L} \\ B_{\ell,\eta} \in B_\Gamma}} \int_{B_{\ell,\eta} \cap \Gamma} [\![ y^{\ell,\eta} \eta ]\!]^2 \, dS . \qquad (3.4)$$

The total energy is defined as

$$\mathcal{E}^D\{y\} = \sum_{\eta \in R} \mathcal{E}_\eta\{y\},$$

where

$$\mathcal{E}_\eta\{y\} = E^a_{\Omega_a,\eta}\{y\} + E^{a,cb}_{\Omega_*,\eta}\{y\} + \tilde{E}_{\Gamma,\eta}\{y\} .$$

Despite the fact that we allow discontinuities, the total energy $\mathcal{E}^D = \sum_{\eta \in R} \mathcal{E}_\eta$ is consistent (ghost-force free) [43]. Designing such consistent coupled energies is one of the few well defined problems in multiscale modelling. The methodology introduced in [43] leads to the systematic design of *ghost-force-free* couplings in two and three dimensions for pair potentials. A previous breakthrough is due to Shapeev [55] who introduced the first consistent methods in two dimensions, see also [40, 42]. The methods introduced in [43] resolved other open algorithmic design issues as well, such as the construction of consistent couplings of arbitrary high-order of accuracy.

The work [34] is devoted to the analysis of the discontinuous interface coupling methods. It contains the analysis of the energy consistency of an altered version of the above coupled method as well. The design of the new methods introduced in [34] was motivated by the error analysis. The key idea is that without specifying the interface terms, the analysis identifies two types of terms: (a) terms which are $O(\varepsilon^2)$ and vanish when $y = y_F$ and (b) terms which are $O(1)$ even for $y = y_F$. However, the terms in (b) are explicit and they have an appropriate structure which motivates the correct introduction of interface energy terms in order to eliminate their effect. The proof that the coupled energy introduced above is a second order approximation to the Cauchy-Born energy was proved in [34] as follows

**Theorem 3.4** (Energy Consistency). *Let $y$ be a smooth function, and $\mathcal{E}^D\{y\}$ be the coupled energy, then there exists a constant $M_E = M_E(y)$, such that*

$$|\mathcal{E}^D\{y\} - \Phi^{CB}(y)| \le M_E \varepsilon^2 .$$

Further, the variational consistency error for the coupled method is bounded by $(\varepsilon^2 + \varepsilon^{2-\frac{1}{p}})$ in the discrete $W^{-1,p}$ norm, as follows

**Theorem 3.5.** *Let $y$ be a smooth function; then the atomistic variation $\langle D\Phi^{CB}(y), v \rangle$ approximates the variation of the coupled discontinuous method $\langle D\mathcal{E}^D\{y\}, v \rangle$ in the*

*sense that there exists a constant $M_V = M_V(y,p)$, $1 \le p \le \infty$, independent of $v$, such that*

$$\left| \langle D\mathcal{E}^D\{y\}, v \rangle - \langle D\Phi^{CB}(y), v \rangle_\varepsilon \right| \le M_V \left( \varepsilon^2 + \varepsilon^{2-1/p} \right) |v|_{W^{1,p}(\Omega)}.$$

# 4 A cell interaction problem and phase transitions

Aiming at discovering the mechanisms of cell interactions within a fibrin medium we would like to approximate a variational problem involving a non strict rank-one convex strain energy function, regularised by a higher order term. The strain energy function models the mechanical response of the extracellular space (ECM). Typical biological tissue are composed of cells surrounded by the extracellular space, which is mainly composed of collagen fibers. Cells are attached onto the ECM fibers through proteins known as adhesion molecules. Through these molecules, cells can detect mechanical alterations to their microenvironment and can pull the surrounding fibers. Cells typically deform the matrix by actively contracting. These tractions can be high enough to create distinct spatial patterns [32, 57, 47], i.e. tissue morphogenesis. In [31] the theory of non-linear elasticity has been used to define an appropriate strain energy which models the cell interactions as phase transitions. To this end, consider the problem of minimizing the total potential energy

$$\Psi[\boldsymbol{u}] = \int_\Omega W(\nabla \boldsymbol{u}(\boldsymbol{x})) + \frac{\varepsilon^2}{2} |\nabla \nabla \boldsymbol{u}(\boldsymbol{x})|^2, \tag{4.1}$$

where $\boldsymbol{u} \in H^2(\Omega)^2$ and $\boldsymbol{u}$ satisfies some appropriate boundary conditions, $\varepsilon > 0$ is a fixed real number and $\Omega \subset \mathbb{R}^2$ is a two dimensional open connected set with Lipschitz boundary. We assume the following upper and lower bounds for the strain energy function $W$:

$$c_0 \left( |\boldsymbol{1} + \nabla \boldsymbol{u}|^2 - c_1 \right) \le W(\nabla \boldsymbol{u}) \le c_2 \left( |\boldsymbol{1} + \nabla \boldsymbol{u}|^m + c_3 \right), \tag{4.2}$$

for some $m \in \mathbb{N}$ and $c_0, c_1, c_2, c_3$ are positive constants. We encode boundary conditions in the following set:

$$\mathbb{A}(\Omega) = \{ \boldsymbol{u} \in H^2(\Omega)^2 : \boldsymbol{u} = \boldsymbol{g}, \text{ for } \boldsymbol{g} \in H^3(\Omega) \} \tag{4.3}$$

where $\boldsymbol{u} = \boldsymbol{g}$ on $\partial \Omega$ in the sense of trace.

Now, the minimization problem can be defined as:

$$\inf\{\Psi[\boldsymbol{u}] : \boldsymbol{u} \in \mathbb{A}(\Omega)\}. \tag{4.4}$$

Next assume for simplicity that the domain is polygonal and, henceforth, $T_h$ denotes the shape regular triangulation of the domain with mesh size $h$. To approximate the solution of the minimization problem (4.4) we use the discrete space of continuous piecewise polynomial functions over $T_h$,

$$V_h^q(\Omega) = \{v \in C^0(\Omega) : v\big|_K \in \mathbb{P}_q(K), K \in T_h\}, \quad q \in \mathbb{N}. \tag{4.5}$$

The set of the internal mesh edges will be called $E_h^i$ and the length of an edge $e$ is denoted by $h_e$.

A direct discretization of the minimization problem (4.4) would require an approximation space, a subspace of $H^2(\Omega) \times H^2(\Omega)$. This means that, for conforming finite elements, we would require $C^1$ continuity at the interfaces, i.e. across element internal boundaries. It is well known that the construction of elements that ensure $C^1$ continuity is quite complex. Here we adopt to our problem an alternative approach based on the discontinuous Galerkin formulation. Our approximations will be sought on $V_h^q(\Omega)^2$; however, the energy functional should be modified to account for possible discontinuities of normal derivatives at the element faces. The appropriate modification of the energy functional proposed below is motivated by the analysis in [43]; the resulting bilinear form of the biharmonic operator obtained via the first variation, will be the form of the $C^0$ discontinuous Galerkin method for the linear biharmonic problem, introduced in [11].

The discretized functional for $\boldsymbol{u}_h \in V_h^q(\Omega)^2$ and $q \geq 2$ has the form:

$$\begin{aligned}
\Psi_h[\boldsymbol{u}_h] = &\int_\Omega \Big[W(\nabla\boldsymbol{u}_h) + \varepsilon^2 \Big(\frac{1}{2}\sum_{K\in T_h}\int_K |\nabla\nabla\boldsymbol{u}_h|^2 \\
&- \sum_{e\in E_h^i}\Big[\int_e \{\!\!\{\nabla\nabla\boldsymbol{u}_h\}\!\!\}\cdot[\![\nabla\boldsymbol{u}_h\otimes\boldsymbol{n}_e]\!] + \frac{\alpha}{h_e}\int_e |[\![\nabla\boldsymbol{u}_h]\!]|^2\Big]\Big).
\end{aligned} \tag{4.6}$$

Note that the higher order terms, terms multiplied by $\varepsilon$, have also a penalty parameter $\alpha$, which is a stabilisation parameter. From now on we assume that $\alpha$ is large enough, see [30] for details. Similarly, to the continuous problem we encode boundary conditions in the following set:

$$\mathbb{A}_h^q(\Omega) = \{\boldsymbol{u}_h \in V_h^q(\Omega)^2 : \boldsymbol{u}_h\big|_{\partial\Omega} = \boldsymbol{g}_h\big|_{\partial\Omega}\}, \tag{4.7}$$

where $\boldsymbol{g}_h \to \boldsymbol{g}$ in $L^2(\partial\Omega)^2$ as $h \to 0$, $\boldsymbol{g}$ is given in (4.3). So, we have to solve the corresponding discrete minimization problem

$$\inf\{\Psi_h[\boldsymbol{u}_h] : \boldsymbol{u}_h \in \mathbb{A}_h^q(\Omega)\}. \tag{4.8}$$

A computational result, adopting the above numerical scheme, can be seen in Figure 7, where the evolving phase transitions are regularised by the parameter $\varepsilon$. The above numerical scheme is used for the detailed computational experiments in [31]. The agreement of the computational model to a series of experiments is remarkable and reveals the real mechanisms of cell interactions, see [31] for details.

It is natural therefore to mathematically justify the appropriateness of this discretisation scheme compared to (4.1). To this end, we will use the theory of $\Gamma$-convergence to compare the continuous and the discretised energies for fixed $\varepsilon$ and $h \to 0$. Here we study the convergence of discrete almost absolute minimizers. Specifically, let $(\boldsymbol{u}_h)$ be a sequence of almost absolute minimizers for the discretized energy functional $\Psi_h$, namely

$$\Psi_h[\boldsymbol{u}_h] = \inf_{\boldsymbol{w}_h \in \mathbb{A}_h^q(\Omega)} \Psi_h[\boldsymbol{w}_h] + \varepsilon_h, \tag{4.9}$$

for some sequence $(\varepsilon_h)$ such that $\varepsilon_h \to 0$, as $h \to 0$. Equation (4.9) indicates that, for a fixed $h$, $\boldsymbol{u}_h$ is an almost absolute minimizer of $\Psi_h$. Therefore, it is natural to ask, if $\boldsymbol{u}_h \to \boldsymbol{u}$ in $H^1(\Omega)^2$ as $h \to 0$, then is $\boldsymbol{u}$ an absolute minimizer of the continuous problem (4.1)? To answer this question first we reformulate the higher order terms of the discrete energy functional in terms of lifting operators [8, 12], which will not be presented here. Then, we prove equi-coercivity of the reformulated discrete energy $\Psi_h$ and the $\Gamma-$convergence of $\Psi_h$ to the continuous energy functional $\Psi$. Finally, using discrete Sobolev embeddings, [20, 21, 14], we show the convergence result of the almost absolute discrete minimizers. A detailed study can be found in [30].

For the discrete function it holds that $\boldsymbol{u}_h \in H^1(\Omega)^2$ and also $\boldsymbol{u}_h\big|_K \in H^2(K)^2$, for all $K \in T_h$. Therefore, we define the broken Sobolev seminorm for $\boldsymbol{w} \in V_h^q(\Omega)^2$:

$$|\boldsymbol{w}|^2_{H^2(\Omega,T_h)} := \sum_{K \in T_h} \int_K |\nabla\nabla\boldsymbol{w}|^2 + \sum_{e \in E_h^i} \frac{1}{h_e} \int_e |[\![\nabla\boldsymbol{w}]\!]|^2. \tag{4.10}$$

A fundamental property of the discrete energy functional is the *equi-coercivity*. If equi-coercivity holds then a uniformly bounded discrete energy implies that the discrete function $\boldsymbol{u}_h$ is uniformly bounded in $H^1(\Omega)$-norm and in the broken Sobolev $H^2(\Omega, T_h)$-seminorm. These bounds are necessary to prove the $\Gamma$-convergence result. Also, from these bounds we can show that the limit of $\boldsymbol{u}_h$ belongs to $H^2(\Omega)^2$ (regularity of the limit). The proposition of equi-coercivity follows below.

**Proposition 4.1** (Equi-coercivity). *Let $(\boldsymbol{u}_h)_{h>0}$ be a sequence of displacements in $V_h^q(\Omega)^2$ such that for a constant $C > 0$ independent of $h$ it holds that*

$$\Psi_h[\boldsymbol{u}_h] \leq C.$$

*Then the there exists a constant $C_1 > 0$ such that*

$$|\boldsymbol{u}_h|^2_{H^2(\Omega, T_h)} \leq C_1. \tag{4.11}$$

*In addition, if $\boldsymbol{u}_h \in \mathbb{A}^q_h(\Omega)$ then*

$$\|\boldsymbol{u}_h\|_{H^1(\Omega)^2} \leq C_2, \tag{4.12}$$

*for a positive constant $C_2$, where $C_1, C_2$ are independent of $h$.*

We will say that $\Psi$ is the $\Gamma$-limit of the sequence $(\Psi_h)$ if the $\limsup$ and the $\liminf$ inequalities are satisfied, [10, 17], as it is described in the next theorem. A $\Gamma$-convergence result for discrete surface functionals involving high gradients using conforming spaces can be found in [7]. The fact that in our case we use finite element spaces with only $H^1$ regularity is the main source of technical difficulties. The next results are proved in [30].

**Theorem 4.2** ($\Gamma-$convergence.). *Let the strain energy function $W$ satisfy the upper and lower bounds of equation (4.2). Then the following properties hold:*

*(i) (The $\limsup$ inequality.) For all $\boldsymbol{u} \in \mathbb{A}(\Omega)$, there exists a sequence $(\boldsymbol{u}_h)_{h>0}$ with $\boldsymbol{u}_h \in \mathbb{A}^q_h(\Omega)$, such that $\boldsymbol{u}_h \to \boldsymbol{u}$ in $H^1(\Omega)^2$ and*

$$\Psi[\boldsymbol{u}] \geq \limsup_{h \to 0} \Psi_h[\boldsymbol{u}_h]. \tag{4.13}$$

*(ii) (The $\liminf$ inequality.) For all $\boldsymbol{u} \in \mathbb{A}(\Omega)$ and all sequences $(\boldsymbol{u}_h) \subset \mathbb{A}^q_h(\Omega)$ such that $\boldsymbol{u}_h \to \boldsymbol{u}$ in $H^1(\Omega)$ the following holds*

$$\Psi[\boldsymbol{u}] \leq \liminf_{h \to 0} \Psi_h[\boldsymbol{u}_h]. \tag{4.14}$$

Next we would like to derive some compactness properties. We would like to show that bounded sequences of the discrete function in the $H^1(\Omega)$-norm and in the $H^2(\Omega, T_h)$-seminorm are relatively compact in $W^{1,p}(\Omega)^2$, for $p \in [1, +\infty)$. Using related discrete compactness results, see [39, 25, 20, 14], one can prove a discrete version of the Rellich-Kondrachov Theorem for our discrete space.

**Proposition 4.3** (Discrete Rellich-Kondrachov). *Let a sequence $(\boldsymbol{u}_h) \subset V^q_h(\Omega)^2$ be bounded, for a constant $C > 0$, as*

$$\|\boldsymbol{u}_h\|_{H^1(\Omega)} + |\boldsymbol{u}_h|_{H^2(\Omega, T_h)} < C, \quad \text{for all } h > 0. \tag{4.15}$$

*Then $(\boldsymbol{u}_h)$ is relatively compact in $W^{1,p}(\Omega)^2$ for $1 \leq p < +\infty$, i.e. there exists a $\boldsymbol{u} \in W^{1,p}(\Omega)^2$ such that*

$$\boldsymbol{u}_h \to \boldsymbol{u} \quad \text{in } W^{1,p}(\Omega)^2, \tag{4.16}$$
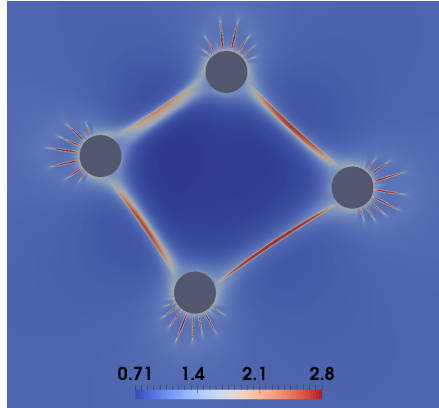
*up to a subsequence.*

**Fig. 7:** Density in the deformed configuration. The circular cavities contract $50\%$, i.e. their radius is reduced from $r$ to $r/2$, deforming the surrounding material. Every circular cavity is connected through tracts of high density with its two nearest neighbors. These tracts correspond to a compressed phase. This computation simulates contracting explants. The formation of the tracts is in agreement with experimental results, see [57]. For this simulation the regularization parameter has the value $\varepsilon = 0.0025r$.

Combining the above results we conclude to the following

**Theorem 4.4** (Convergence of discrete almost absolute minimizers). *Let $(\boldsymbol{u}_h) \subset \mathbb{A}_h^q(\Omega)$ be a sequence of almost absolute minimizers of $\Psi_h$, i.e.,*

$$\Psi_h[\boldsymbol{u}_h] = \inf_{\boldsymbol{w}_h \in \mathbb{A}_h^q(\Omega)} \Psi_h[\boldsymbol{w}_h] + \varepsilon_h, \tag{4.17}$$

*for some sequence $(\varepsilon_h)$ such that $\varepsilon_h \to 0$, as $h \to 0$. If $\Psi_h[\boldsymbol{u}_h]$ is uniformly bounded then, up to a subsequence, there exists $\boldsymbol{u} \in \mathbb{A}(\Omega)$ such that*

$$\boldsymbol{u}_h \to \boldsymbol{u}, \quad in \ H^1(\Omega)^2, \tag{4.18}$$

*and*

$$\Psi[\boldsymbol{u}] = \min_{\boldsymbol{w} \in \mathbb{A}(\Omega)} \Psi[\boldsymbol{w}]. \tag{4.19}$$

# 5 Computation of measure-valued solutions for hyperbolic problems

In many problems, such as (2.1), the behaviour of approximations of solutions is not always certain. Uncertainties in the solution can be caused, for instance, by the initial data, or the parameters appearing in the model. One of the reasons is that in practice it is impossible to obtain exact measurements. Hence, we are interested in studying and computing solutions that deal with the problem of uncertainty in PDEs. Furthermore, a similar problem from a mathematical perspective relates to statistical inference on the solutions when we study an assembly of variable data of the model. Statistics is a discrete endeavour and when it comes to complicated models such as nonlinear PDEs there are more than one (continuous) mathematical settings to formulate problems. A possible way to access uncertainty in nonlinear hyperbolic systems is to use the concept of measure-valued or statistical solutions, [38, 28, 19, 26, 2, 3, 1].

*Measure valued solutions.* Let now $\mathbf{M}^+(\mathbb{R}^m)$ be the set of all positive Radon measures on $\mathbb{R}^m$, and $\mathbf{M}^{\mathbb{P}}(\mathbb{R}^m) = \{\mu \in \mathbf{M}^+(\mathbb{R}^m), \mu(\mathbb{R}^m) = 1\}$ the corresponding set of probability measures. We call *Young measure* a weakly* measurable mapping from $\Omega$ into $\mathbf{M}^{\mathbb{P}}(\mathbb{R}^m)$. The set of all Young measures is denoted by $\mathbf{Y}(\Omega, \mathbb{R}^m)$. A parametrised measure $\mu \in \mathbf{Y}(\Omega, \mathbb{R}^m)$ is said to be a measure-valued solution of the conservation law (2.1) if, [22],

$$\int_{\Omega} \big(\langle id, \mu_{x,t}\rangle \cdot \phi_t + \langle A, \mu_{x,t}\rangle \cdot \phi_x\big)dxdt + \int_{\mathbb{R}} u_0 \cdot \phi(0, x)dx = 0, \qquad (5.1)$$

for all $\phi \in C_0^\infty(\overline{\Omega})$ where by $\langle A, \mu_{x,t}\rangle$ we denote

$$\langle A, \mu_{x,t}\rangle = \int_{\mathbb{R}^m} A(\lambda)d\mu_{x,t}(\lambda).$$

Note that for notational connivence in this section, we denote the flux function of the conservation law by $A$ as opposed to $F$ or $f$ usually used. In a similar fashion as for weak solutions, an *entropy measure-valued solution* satisfies the additional relation

$$\int_{\Omega} \big(\langle \eta, \mu_{x,t}\rangle \cdot \phi_t + \langle Q, \mu_{x,t}\rangle \cdot \phi_x\big)dxdt + \int_{\mathbb{R}} u_0 \cdot \phi(0, x)dx \geq 0, \qquad (5.2)$$

for all $\phi \in C_0^\infty(\Omega)$ with $\phi \geq 0$, where $\eta$ is convex and $(\eta, Q)$ an entropy entropy-flux pair, [16]. The notion of entropic measure-valued solutions which was originally proposed by DiPerna [22] is rather weak when non-atomic measures are considered.

A manifestation of this fact is the loss of uniqueness, even in the scalar case, when non-atomic measures were allowed in the initial data, [16]; an alternative definition was proposed recently in [27] which leads to a uniqueness result within a certain class.

*Statistical methods through approximate Young measures.* Our aim is to develop a new approach to the computation of measure valued solutions and to quantify uncertainties for nonlinear hyperbolic problems, based on two key ingredients : *approximate Young measures* and *kinetic models*. We show below, following [29], that approximate Young measures, [54, 50], give rise in a natural way to discrete kinetic models. In the scalar case the kinetic formulation of conservation laws, [41, 51], provides an interesting connection to parametrised Young measures and to compensated compactness. This connection was further developed in [49, 52, 51] for scalar laws and in [18] where kinetic formulations were the analytical basis to study conservation laws with stochastic forcing. Our aim is to build an algorithmic approach which leads to efficient schemes for the computation of measure valued solutions and to UQ starting from the scalar case. These schemes are very different from existing sampling approaches, since they rely on solving discretised kinetic models with prescribed approximate defect measures on the right hand side. Kinetic formulations are used in a different way in [19].

Suppose that $h > 0$ is a mesh discretisation parameter, let $S \subset \mathbb{R}^m$, and $S_h$ is a finite dimensional subspace of $C(S)$. We assume that there exist a continuous linear projector $P_h : L^1(\Omega; C_0(S)) \rightarrow L^1(\Omega; S_h) = P_h(L^1(\Omega; C(S)))$. Let further $\mathbf{Y}_h(\Omega, S)$ be the set of all Young measures which map $\Omega$ into $(S_h)^*$. One can define $\mathbf{Y}_h(\Omega, S)$, the space of approximate Young measures, through the following procedure, see [54] for details. Given $\mu \in \mathbf{Y}(\Omega, S)$, $\mu$ is approximated by a $\bar{\mu} \in \mathbf{Y}_h(\Omega, S)$ defined as

$$\int_\Omega \langle \phi, \bar{\mu}_{x,t} \rangle dx dt = \int_\Omega \langle P_h \phi, \mu_{x,t} \rangle dx dt, \tag{5.3}$$

for all $\phi \in L^1(\Omega; C(S))$. To fix ideas, consider $m = 1$, $S_h$ being the standard finite element space of continuous piecewise linear functions, and $P_h$ the standard interpolation operator,

$$P_h(\phi(t, x, \xi)) = \sum_{i=1}^n \phi(x, t, \xi_i) v_i(\xi). \tag{5.4}$$

Here, $\{v_i\}_{i=1}^n$ are the hat-basis elements of $S_h$ and $\{\xi_i \in S\}_{i=1}^n$ are the mesh points. It is essential now to see the form of the approximate measure:

$$\int_\Omega \langle \phi, \bar{\mu}_{x,t} \rangle dxdt = \int_\Omega \langle \sum_{i=1}^n \phi(x,t,\xi_i) v_i(\xi), \mu_{x,t} \rangle dxdt$$

$$= \sum_{i=1}^n \int_\Omega \phi(x,t,\xi_i) \langle v_i(\xi), \mu_{x,t} \rangle dxdt = \sum_{i=1}^n \int_\Omega \alpha_i(x,t) \int_S \phi(x,t,\lambda) d\delta_{\xi_i}(\lambda) dxdt$$

$$= \int_\Omega \int_S \phi(x,t,\lambda) d[\sum_{i=1}^n \alpha_i(x,t)\delta_{\xi_i}(\lambda)] dxdt = \int_\Omega \langle \phi, \sum_{i=1}^n \alpha_i(x,t)\delta_{\xi_i} \rangle dxdt$$

for all $\phi \in L^1(\Omega; C(S))$ where $\alpha_i(x,t) = \langle v_i, \mu_{x,t} \rangle$ and $\delta_x$ is the Dirac measure at $x$. Therefore,

$$\bar{\mu}_{x,t} = \sum_{i=1}^n \alpha_i(x,t)\delta_{\xi_i}. \tag{5.5}$$

In other words, expression (5.5) indicates that such approximations of a Young measure $\mu$ is reduced to the evaluation of the action of $\mu$ on every basis function $v_i$ of the space $S_h$. As the functions $\alpha_i$ determine $\bar{\mu}$, the approximating schemes defined below will have as unknowns $\alpha_i$, in a form of a PDE system.

We can now proceed to the computation of approximate measure-valued solutions. Substituting $\mu$ in expression (5.1) with $\bar{\mu}$ and supposing temporarily that $u_0 = 0$ one leads to the approximating scheme

$$\int_\Omega \left( \langle id, \bar{\mu}_{x,t} \rangle \cdot \phi_t + \langle A, \bar{\mu}_{x,t} \rangle \cdot \phi_x \right) dxdt = 0,$$

or,

$$\int_\Omega \left( \langle id, \sum_{i=1}^n \alpha_i(x,t)\delta_{\xi_i} \rangle \cdot \phi_t + \langle A, \sum_{i=1}^n \alpha_i(x,t)\delta_{\xi_i} \rangle \cdot \phi_x \right) dxdt = 0$$

Thus, one may conclude that the evolution of $\alpha_i$ is dictated by the partial differential equation

$$\sum_{i=1}^n \xi_i \alpha_i(x,t)_t + \sum_{i=1}^n A(\xi_i)\alpha_i(x,t)_x = 0. \tag{5.6}$$

Expression (5.6) now will constitute the cornerstone of our approach. However, some remarks are in order: although (5.6) has to be satisfied, this equation does not constitute a complete PDE system, and we need to quest a system for $\alpha_i$ at another level which will be complete and will imply (5.6). An indicative such system can be

$$\partial_t \alpha_i(x,t)\xi_i + \partial_x \alpha_i(x,t)A(\xi_i) = M_i, \quad i = 1, \ldots, n, \tag{5.7}$$

where the source functions $M_i$ are given and satisfy $\sum_i M_i = 0$. Such equations are reminiscent of discrete kinetic models, though one has to specify appropriately $M_i$. Similarly, as in the case of weak solutions where we had to impose additional entropy inequalities in order to distinguish a physically relevant solution out of infinitely many weak solutions, in this case too, we have to enrich (5.6) in a right way with additional information in order to compute a meaningful solution of (5.1). This can be realised through the setting of the *kinetic formulation* of conservation laws, [41, 51]. In fact, to motivate the design of appropriate discrete kinetic models leading to (5.6) we will seek appropriate discretisations of functions $f(t, x, \xi)$ of the kinetic formulation: A function $f(t, x, \xi) \in L^\infty(0, +\infty; L^1(\mathbb{R}^2))$ is called a *generalised kinetic solution of the scalar conservation law,* [51], with initial data $f_0$, if for all $\phi \in D([0, +\infty) \times \mathbb{R} \times \mathbb{R})$ we have

$$
\int_0^\infty \int_{\mathbb{R}^{m+1}} f(t, x, \xi) \left[ \frac{\partial \phi(t, x, \xi)}{\partial t} + A'(\xi) \frac{\partial \phi(t, x, \xi)}{\partial x} \right] dx d\xi dt
$$

$$
= \int_0^\infty \int_{\mathbb{R}^{m+1}} m(t, x, \xi) \frac{\partial \phi(t, x, \xi)}{\partial \xi} dx d\xi dt - \int_{\mathbb{R}^{m+1}} f_0(x, \xi) \phi(0, x, \xi) dx d\xi,
$$

(5.8)

where $m$ is a bounded nonnegative measure on $((0, +\infty) \times \mathbb{R} \times \mathbb{R})$ and additionally it holds that

$$
|f(t, x, \xi)| = sgn(\xi) f(t, x, \xi) \leq 1, \tag{5.9a}
$$

$$
f = \int_{\mathbb{R}} \chi_\lambda(\xi) d\nu_{x,t}(\lambda). \tag{5.9b}
$$

Here, $\nu_{x,t}$ is a Young measure associated to $f$ and $\chi_\lambda$ is given by

$$
\chi_\lambda(\xi) = \begin{cases} 1 \text{ if } 0 < \xi \leq \lambda \\ -1 \text{ if } \lambda \leq \xi < 0 \\ 0 \text{ otherwise.} \end{cases}
$$

*Kinetic functions and approximate Young measures.* At this point, notice that the right term of (5.18) plays a key role. Specifically, the defect measure $m$ might provide the additional information we are looking for leading to a chosen measure-valued solution. Suppose now that the approximate Young measure $\bar{\nu}_{x,t} = \sum_{i=1}^{n} \alpha_i(x, t) \delta_{\xi_i}$ approximates

$\nu_{x,t}$. We see then

$$f(t, x, \xi) \approx \bar{f}(t, x, \xi) = \int_{\mathbb{R}} \chi_\lambda(\xi) d\bar{\nu}_{x,t} = \int_{\mathbb{R}} \chi_\lambda(\xi) d[\sum_{i=1}^{n} \alpha_i(x, t)\delta_{\xi_i}(\lambda)]$$

$$= \sum_{i=1}^{n} \alpha_i(x, t) \int_{\mathbb{R}} \chi_\lambda(\xi) d\delta_{\xi_i}(\lambda) = \sum_{i=1}^{n} \alpha_i(x, t)\chi_{\xi_i}(\xi) = \sum_{i=1}^{n} \bar{f}_i,$$

where $\bar{f}_i = \alpha_i(x, t)\chi_{\xi_i}(\xi)$. Therefore, one can define the approximate model

$$\sum_{i=1}^{n} \frac{\partial \bar{f}_i}{\partial_t} + \sum_{i=1}^{n} A'(\xi) \frac{\partial \bar{f}_i}{\partial_x} = \frac{\partial \bar{m}}{\partial \xi} \qquad (5.10)$$

where $\bar{m}$ is an approximation of measure $m$. We observe now

$$\int_{\mathbb{R}} \frac{\partial \bar{f}_i}{\partial_t} + A'(\xi) \frac{\partial \bar{f}_i}{\partial_x} \, d\xi = \partial_t \alpha_i(x, t) \int_{\mathbb{R}} \chi_{\xi_i}(\xi) d\xi + \partial_x \alpha_i(x, t) \int_{\mathbb{R}} A'(\xi)\chi_{\xi_i}(\xi)d\xi$$

$$= \xi_i \partial_t \alpha_i(x, t) + A(\xi_i)\partial_x \alpha_i(x, t). \qquad (5.11)$$

Therefore, by integrating (5.10) we conclude that

$$\sum_{i=1}^{n} \partial_t \alpha_i(x, t)\xi_i + \sum_{i=1}^{n} \partial_x \alpha_i(x, t)A(\xi_i) = \int_{\mathbb{R}} \frac{\partial \bar{m}}{\partial \xi} d\xi = 0. \qquad (5.12)$$

In addition, piecewise integration leads to

$$\int_{\mathbb{R}} \frac{\partial \bar{m}}{\partial \xi} d\xi = \sum_{i=1}^{n-1} \bar{m}(x, t, \xi_{i+1}) - \bar{m}(x, t, \xi_i) = 0. \qquad (5.13)$$

We can see now, that expression (5.12) is of the form (5.6). Motivated by the above discussion one can formulate alternative approximating schemes in order to compute the unknowns $\alpha_i(x, t)$. Probably the simplest case is the following: For $i = 1, \ldots, n-1$ in each interval $(\xi_i, \xi_{i+1})$ find $\alpha_i(x, t)$ such that

$$\partial_t \alpha_i(x, t)\xi_i + \partial_x \alpha_i(x, t)A(\xi_i) = \bar{m}(x, t, \xi_{i+1}) - \bar{m}(x, t, \xi_i). \qquad (5.14)$$

As it is obvious the implementation of the above system requires that the measure $\bar{m}$ is known. We can observe now that in kinetic models for conservation laws with small diffusion the defect measure can be explicitly computed, [15]. Typically, it contains a diffusion term of the kinetic function $f(t, x, \xi)$ as well. In fact, [15, 44], the kinetic formulation of

$$\partial_t u + \partial_x A(u) = \epsilon u_{xx}, \quad x \in \mathbb{R}, \ t > 0, \qquad (5.15)$$

is

$$\frac{\partial \chi_u(\xi)}{\partial t} + A'(\xi)\frac{\partial \chi_u(\xi)}{\partial x} - \epsilon\frac{\partial^2 \chi_u(\xi)}{\partial x^2} = \epsilon\left(\frac{\partial \delta(\xi - u)}{\partial \xi}\left(\frac{\partial u}{\partial x}\right)^2\right) = \frac{\partial m^\epsilon}{\partial \xi}. \quad (5.16)$$

Motivated by the above discussion, and the fact that we would like to include in our approximate scheme artificial diffusion, we are led to the following approximating model: Let first $\widetilde{u}$ be defined through

$$\widetilde{u} = \int_{\mathbb{R}} \lambda d\bar{\nu}_{x,t}(\lambda) = \int_{\mathbb{R}} \lambda d\sum_{i=1}^{n}\alpha_i(x,t)\delta_{\xi_i} = \sum_{i=1}^{n}\alpha_i(x,t)\xi_i.$$

For fixed $x_0$, we consider $\bar{\delta}(\xi - x_0)$ to be a compactly supported smooth Gaussian-like approximation of $\delta(\xi - x_0)$. Then one can define the discrete kinetic model yielding $\alpha_i$ through

$$\xi_i\alpha_i(x,t)_t + A(\xi_i)\alpha_i(x,t)_x = \epsilon\alpha_i(x,t)_{xx}$$
$$+ \bar{m}^\epsilon(x,t,\xi_{i+1}) - \bar{m}^\epsilon(x,t,\xi_i), \quad (5.17)$$

where $\bar{m}^\epsilon(t,x,\xi) = \epsilon\left(\bar{\delta}(\xi - \widetilde{u})\,|\widetilde{u}_x|^2\right)$. We observe that at least formally, as $\epsilon \to 0$, the model (5.17) is of the form (5.14). Obviously, the choice of the models is indicative and it is open to find the schemes which will produce the most efficient approximations. *Uniquennes.* Although it is quite natural to design schemes which induce a form of artificial diffusion, a key question is, if it is possible to have some guarantees that we compute in the limit a unique measure. A partial result in this direction is stated below. We need first to extend the definition of generalised kinetic solutions to include small diffusion. To this end, a function $f(t,x,\xi) \in L^\infty(0,+\infty; L^1(\mathbb{R}^2))$ is called a *generalized kinetic solution of the viscous scalar conservation law* with *initial data $f_0$,* if for all $\phi \in D([0,+\infty) \times \mathbb{R} \times \mathbb{R})$ we have

$$\int_0^\infty \int_{\mathbb{R}^{m+1}} f(t,x,\xi)\left[\frac{\partial\phi(t,x,\xi)}{\partial t} + A'(\xi)\frac{\partial\phi(t,x,\xi)}{\partial x}\right]dxd\xi dt$$

$$= -\int_0^\infty \int_{\mathbb{R}^{m+1}} B_\varepsilon(x)\frac{\partial f(t,x,\xi)}{\partial x}\,\frac{\partial\phi(t,x,\xi)}{\partial x}dxd\xi dt$$

$$+ \int_0^\infty \int_{\mathbb{R}^{m+1}} m'(t,x,\xi)\frac{\partial\phi(t,x,\xi)}{\partial \xi}dxd\xi dt - \int_{\mathbb{R}^2} f_0(x,\xi)\phi(0,x,\xi)dxd\xi$$

$$(5.18)$$

where $m'$ is a given bounded nonnegative measure on $((0,+\infty) \times \mathbb{R} \times \mathbb{R})$, $B_\varepsilon(x) \geq 0$, and

$$|f(t,x,\xi)| = sgn(\xi)f(t,x,\xi) \leq 1, \quad (5.19a)$$

$$f = \int_{\mathbb{R}} \chi_\lambda(\xi) d\nu_{x,t}(\lambda). \tag{5.19b}$$

The next result essentially states that all viscous generalised kinetic functions have the same limit as soon as $\|B_\epsilon\|_{L^\infty} \to 0$, and the defect measures satisfy a dissipative structural assumption. Note at this point the similarity with the scalar problem (2.1) where we obtain the unique entropy solution through the vanishing viscosity limit. The assumption for the measures stated below is understood via regularisation and we are not precise regarding the smoothness assumptions on the viscosity coefficients $B_\epsilon$.

**Theorem 5.1.** *Assume that $f$ is a solution of* (5.18) *and let $\bar{f}$ a viscous generalised kinetic solution of* (5.18) *corresponding to $\bar{B}_\varepsilon(x), \bar{m}'$, and $\bar{\nu}$. Furthermore, suppose that the initial data and the solutions have compact support with $\bar{f}(0, x, \xi) = f(0, x, \xi)$. In addition to these hypothesis, assume that the defect measures $m'$ and $\bar{m}'$ satisfy, up to regularisation,*

$$\int_0^T \int_{\mathbb{R}} \int_{\mathbb{R}} m' - \bar{m}' \, d(\nu - \bar{\nu}) dx \, d\xi \, dt \leq 0, \tag{5.20}$$

*and $m' = 0$ ($\bar{m}' = 0$) if $f = 0$ ($\bar{f} = 0$). Then, as both $\|B\|_{L^\infty}, \|\bar{B}\|_{L^\infty} \to 0$ we have the limit*

$$\|f - \bar{f}\|_{L^2} \to 0.$$

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