1 Research Interests

My long-standing research interests are in the area of nonlinear partial differential equations, hyperbolic conservation laws, calculus of variations and applications of these fields to materials science and nonlinear solid mechanics, with a special interest in problems of dynamic cavitation and fracture in hyperelastic solids. Two of my recently acquired research interests are mathematical biology, with applications to microbial population dynamics, and statistics, with applications to big data and analytics.

2 Past Research

2.1 Variational Schemes for Polyconvex Elastodynamics

In my Ph.D. thesis at the University of Maryland I studied variational methods for solutions to the equations of nonlinear elastodynamics with polyconvex stored energy describing the behavior of hyperelastic materials (rubbers, polymers, soft biological tissues). I achieved two interrelated objectives in my work. I considered the novel variational scheme introduced by S. Demoulini, D.M.A. Stuart and A. Tzavaras [13] that approximates the equations of elastodynamics in three dimensions and established the strong convergence of the time-continuous interpolates constructed in the scheme to the solution of elastodynamics before shock formation (see [29]). Also, I studied the equations describing radial motions of isotropic elastic materials. I constructed a variational approximation scheme that decreases the total mechanical energy and leads to physically realizable motions that avoid interpenetration of matter (see [28]). Handling the impenetrability constraint was the main contribution of the work [28] inspired by the variational method in [13] where such constraint was not taken into account. Below is a detailed description of these works.

2.1.1 Convergence of Variational Schemes for Elastodynamics in 3-d [29]

Polyconvex Elastodynamics. The equations describing the evolution of a continuous hyperelastic medium is the system of nonlinear partial differential equations

$$\frac{\partial^2 y}{\partial t^2} = \operatorname{div} \frac{\partial W}{\partial F}(\nabla y)\,. \tag{2.1}$$

Here $y(x,t) : \mathbb{R}^d \times \mathbb{R}_+ \in \mathbb{R}^d$ describes the motion, $F = \nabla y$ and $v = \partial_t y$ are the deformation gradient and velocity, respectively, and $W : M^{d\times d} \to \mathbb{R}$ is the stored energy function (determining the constitutive properties of the material). Convexity of the stored energy is, in general, incompatible with certain physical requirements and is not a natural assumption. As an alternative, *polyconvex* stored energy is often considered, which means that

$$W(F) = G(F, \operatorname{cof} F, \det F) = G \circ \Psi(F) \quad \text{ with } G(\Xi) \text{ convex.}$$

The system (2.1) is usually recast as a system of twelve conservation laws in the variables $v \in \mathbb{R}^3$ and $F \in \mathbb{R}^9$. In the parlance of conservation law $\eta = \frac{1}{2}|v|^2 + W(F)$ is an entropy with associated entropy flux $q_\alpha = -v_i \frac{\partial W}{\partial F_{i\alpha}}$. The entropy η is not convex (due to the lack of convexity of W) what causes difficulties in applying the standard theory of conservation laws in a direct way.

Variational Method in 3-d. In the novel variational approximation method [13] introduced by S. Demoulini, D.M.A. Stuart and A. Tzavaras the equations of elastodynamics (2.1) are viewed as the constrained evolution of an enlarged system in the variables $v \in \mathbb{R}^3$ and $\Xi = (F, Z, w) \in \mathbb{R}^{19}$; this embedding is motivated by the recently discovered transport identities [47, 13] for null-lagrangians $\Psi(F) \in \mathbb{R}^{19}$. The enlarged system has more variables than the original one, but it is equipped with a convex entropy $\eta(v, \Xi) = \frac{1}{2}|v|^2 + G(\Xi)$. This feature allowed the authors to incorporate standard minimization techniques in the design of the time-discrete approximation method.

The variational method in [13] is based upon time discretization of the enlarged system: given data (v^{n-1}, Ξ^{n-1}) at time step $t = t_{n-1}$ the scheme produces the next iterate via minimization of the convex functional $I[v, \Xi] = \int_\Omega \left\{ \frac{1}{2}|v - v^{n-1}|^2 + G(\Xi) \right\} dx$ over an appropriate admissible set. Marching in time, the scheme constructs a sequence of spatial iterates $\{(v^n, \Xi^n)\}_{n \geqslant 1}$ that solve the corresponding Euler-Lagrange equations,

$$\frac{(v_i^n - v_i^{n-1})}{\Delta t} = \partial_\alpha \Big(\frac{\partial G}{\partial \Xi_A}(\Xi^n) \, \frac{\partial \Psi^A}{\partial F_{i\alpha}}(F^{n-1}) \Big) \,, \quad \frac{\Xi_A^n - \Xi_A^{n-1}}{\Delta t} = \partial_\alpha \Big(\frac{\partial \Psi^A}{\partial F_{i\alpha}}(F^{n-1}) \, v_i^n \Big) \,, \tag{2.2}$$

and generate an entropic measure-valued solution to the equations of elastodynamics (2.1).

My Contribution. Direct Convergence. In my PhD thesis I established the direct convergence of time-continuous interpolates constructed in the time-discrete scheme (2.2) to the solution of elastodynamics before shock formation and provided the error estimate (see [29]). This work was the first step towards fully-discrete numerical method used for practical purposes (eg. computing solutions).

To establish convergence I employed the relative entropy argument (see [12, 14]). I considered the relative entropy,

$$\eta^r \, = \, \tfrac{1}{2}|V^{(\Delta t)} - \bar{V}|^2 + \big[G(\Xi^{(\Delta t)}) - G(\bar{\Xi}) - \mathrm{D}_\Xi G(\bar{\Xi})(\Xi^{(\Delta t)} - \bar{\Xi}) \big] \,,$$

which (essentially) estimates the difference between time-continuous interpolates $V^{(\Delta t)}, \Xi^{(\Delta t)}$ produced by the scheme and a classical solution $\bar{V}, \bar{\Xi}$ of the enlarged system, and derived the energy identity monitoring the time evolution of η^r. The analysis of the identity yielded the main result: if $(\bar{V}, \bar{F})$ are smooth solutions of the elasticity equations (2.1) then

$$\sup_{t \in [0,T]} \Big(\|V^{(\Delta t)} - \bar{V}\|^2_{L^2(\Omega)} + \|\Xi^{(\Delta t)} - \Psi(\bar{F})\|^2_{L^2(\Omega)} + \|F^{(\Delta t)} - \bar{F}\|^p_{L^p(\Omega)} \Big) = O(\Delta t).$$

2.1.2 Variational Scheme for Radial Elasticity [28]

Radial Motions in 3-d Elasticity. A motion of the form $y(x,t) = w(R,t)\frac{x}{R}$, where $R = |x|$, $x \in \mathbb{R}^3$, is called radial. For an elastic material to support radial motions it must be isotropic. The class of such stored energies is characterized to be of the form $W(F) = \Phi(v_1, v_2, v_3)$, where Φ is a symmetric function of the eigenvalues v_1, v_2, v_3 of $\sqrt{F^\top F}$ called principal stretches. A straightforward computation shows that $w(R,t)$ satisfies the partial differential equation of second-order

$$w_{tt} = \frac{1}{R^2} \frac{\partial}{\partial R} \Big(R^2 \frac{\partial \Phi}{\partial v_1}\big(w_R, \frac{w}{R}, \frac{w}{R}\big) \Big) - \frac{1}{R} \sum_{i=2}^{3} \frac{\partial \Phi}{\partial v_i}\big(w_R, \frac{w}{R}, \frac{w}{R}\big) \,. \tag{2.3}$$

To interpret y as a physical motion it is necessary to exclude interpenetration of matter. As a minimum requirement the following condition must be imposed

$$\det F = w_R (w/R)^2 > 0 \,, \quad F = \nabla y \,. \tag{2.4}$$

The equation (2.3) can be recast as a first order system of inhomogeneous balance laws upon introducing the velocity $v = w_t$, radial strain $a = w_R$, and transversal strain $b = \frac{w}{R}$, respectively. Following the usual theory of conservation laws a weak entropy solution is defined to satisfy the entropy inequality

$$\partial_t \Big(\tfrac{1}{2} v^2 + \Phi(a,b,b) \Big) R^2 - \partial_R \Big(R^2 \, v \, \frac{\partial \Phi}{\partial v_1}(a,b,b) \Big) \leq 0 \,. \tag{2.5}$$

Little is known at present concerning the existence of weak solutions for the radial elasticity system (2.3). One additional difficulty is that solutions of (2.3) have to be constructed to satisfy the constraint (2.4) so as to be interpreted as mechanical motions. This constraint is difficult to preserve even in approximating schemes (in [13], for instance, (2.4) was not taken into account).

My Contribution. Variational Scheme for Radial Elasticity. In my PhD thesis I devised a time-discrete variational scheme for solutions to radial elasticity equations (2.3) subject to the uniform stretching at the boundary of the unit ball, $w(1,t) = \lambda$. The scheme preserves the positivity of Jacobians (2.4) and produces iterates that decrease the mechanical energy (see [28]).

To incorporate the constraint (2.4) into the variational scheme I employed a polyconvex stored energy of the specific form

$$\Phi(v_1, v_2, v_3) = \phi(v_1) + \phi(v_2) + \phi(v_3) + g(v_2v_3) + g(v_1v_3) + g(v_1v_2) + h(v_1v_2v_3) \tag{2.6}$$

where ϕ, g and h are convex functions and $h(\delta) \to +\infty$ as $\delta \to 0+$. As in [13], the scheme is based on the transport identities for null-Lagrangians. These transport identities allowed me to view the equation (2.3) as the constrained evolution of first-order system that has four variables $\big(v, \alpha, \beta, \gamma\big)(\rho) = \big(w_t, w^3, w_R/R^2, w^2\big)(R)$, $\rho = R^3$, and admits a convex entropy

$$\eta(v, \Xi) = \tfrac{1}{2}v^2 + G(\Xi)$$

with G convex and $\Xi = \Xi(\alpha, \beta, \gamma, \alpha_\rho, \gamma_\rho, \rho) \in \mathbb{R}^7$ a linear function of its first five arguments.

The extended system is discretized in time using an implicit-explicit method. It is the Euler-Lagrange equations of the variational problem: given v_0, α_0, β_0, γ_0, minimize the convex functional $I[v, \alpha, \beta, \gamma] = \int_0^1 \left\{\frac{1}{2}(v - v_0)^2 + G(\Xi)\right\} d\rho$ over the appropriate set of admissible functions $\mathcal{A}_\lambda$ (which contains the constraint $\alpha'(\rho) = (w_R(\frac{w}{R})^2)|_{R=\rho^{1/3}} > 0$ ensuring the positivity of Jacobians (2.4)). In my work I proved the existence and uniqueness of a minimizer for the functional I over $\mathcal{A}_\lambda$ and that the minimizer was a weak solution to the corresponding Euler-Lagrange equations, that is, a solution of the time-discrete scheme.

Admissible shocks of the elasticity equations are required to dissipate the mechanical energy (equivalently, they must satisfy (2.5)). Accordingly, approximating schemes are expected to respect such behaviors and produce entropy-dissipating solutions in the limit. The variational scheme I developed turns out to satisfy a discrete version of the entropy inequality (2.5).

2.2 Dynamic cavitation in hyperelastic media [17, 30]

Ball [7] in a seminal paper proposed to use continuum mechanics for modeling cavitation and used methods of the calculus of variations and bifurcation theory to construct (radial) cavitating solutions for the equilibrium version of (2.1): There is a critical stretching λ_{cr} such that for $\lambda < \lambda_{cr}$ the homogeneous deformation is the only minimizer of the elastic stored energy; by contrast, for $\lambda > \lambda_{cr}$ there exist nontrivial equilibria corresponding to a (stress-free) cavity in the material with energy less than the energy of the homogenous deformation [7]. In a subsequent important develompent, K.A. Pericak-Spector and S. Spector [41, 42] used the self-similar ansatz, $y(x,t) = \varphi(\frac{R}{t})\frac{t}{R}$, $R = |x|$, $x \in \mathbb{R}^d$, to construct a weak solution for the dynamic problem that corresponds to a spherical cavity emerging at time $t = 0$ from a homogeneously deformed state. The cavitating solution is constructed in dimension $d \geqslant 2$ for special classes of polyconvex energies [41, 42] and sufficiently large initial stretchings. Remarkably, the cavitating solution has lower mechanical energy than the associated homogeneously deformed state from where it emerges [41], and thus provides a striking example of nonuniqueness of entropy weak solutions (for polyconvex energies).

In the article [30] (which complement works [41, 42]) I established various further properties of weak solutions describing dynamic cavitation in isotropic compressible nonlinear elastic materials (with a polyconvex stored energy). For the equations of radial elasticity (2.3) I constructed self-similar weak solutions that describe a cavity emanating from a state of uniform deformation and, for dimensions $d = 2, 3$, showed that cavity formation is necessarily associated with a unique precursor shock. I also studied the bifurcation diagram and did a detailed analysis of the singular asymptotics associated to cavity initiation as a function of the cavity speed $\varphi_0 = \varphi(0)$ of the self-similar profiles. I showed that for stress free cavities the critical stretching associated with dynamically cavitating

solutions coincides with the critical stretching in the bifurcation diagram of equilibrium elasticity [7]. The work [30] (which I view as one of my best results) was a joint project with A. Tzavaras (University of Crete, Greece). The work [17] is a review article with J. Giesselmann (Weierstrass Institute, Germany) and A. Tzavaras which is based on the cavity formation work [30] and the work by Giesselmann and Tzavaras [18] (in which the notion of singular limiting induced from continuum solution is introduced and applied to the problem of cavity formation).

2.3 Relaxation models for hyperbolic balance laws

In the joint projects [31, 32] with K. Trivisa (University of Maryland, College Park) I studied relaxation approximation schemes for systems of hyperbolic balance laws with source terms satisfying a special mechanism that induces weak dissipation in the spirit of Dafermos [11] as well as more general source terms. In the article [31] I presented a general framework for the approximation of systems of hyperbolic balance laws by suitable relaxation systems equipped with a globally defined convex entropy. I provided a direct proof of convergence in the smooth regime for a wide class of physical systems and presented results for systems arising in materials science, where the presence of source terms presents a number of additional challenges. In [32] I introduced a class of relaxation schemes for systems of hyperbolic balance laws in which the regularization effect is achieved by means of a wave operator, a mechanism introduced by Jin and Xin [21] for systems of hyperbolic conservation laws without source terms. I established their stability and convergence to the solution of hyperbolic balance laws before the formation of shocks. Below are the details.

2.3.1 Relative entropy in hyperbolic relaxation of balance laws [31]

Relaxation approximations of hyperbolic balance laws are critical for the investigation of models arising in continuum mechanics and kinetic theory of gases, and serve as a ground stage for the design of numerical schemes for hyperbolic balance laws. Relaxation models are models that approximate the system of balance laws

$$\partial_t u + \sum_{\alpha=1}^{d} \partial_\alpha f_\alpha(u) = g(u), \quad u \in \mathbb{R}^n,\ (x,t) \in \mathbb{R}^d \times \mathbb{R}_+ \tag{2.7}$$

and appear in the form of the extended system

$$\partial_t U + \sum_{\alpha=1}^{d} \partial_\alpha F_\alpha(U) = \frac{1}{\varepsilon} R(U) + G(U), \quad U(x,t) \in \mathbb{R}^N,\ x \in \mathbb{R}^d,\ N > n\,. \tag{2.8}$$

In [31] K. Trivisa and I introduced a general framework for the approximation of systems of hyperbolic balance laws by relaxation systems equipped with a globally defined convex entropy $H(U)$, satisfying

$$\partial_t H(U) + \sum_{\alpha=1}^{d} \partial_\alpha Q_\alpha(U) = \frac{1}{\varepsilon} \mathrm{D}H(U)R(U) + \mathrm{D}H(U)G(U) \quad \text{with} \quad \mathrm{D}H(U)R(U) \leq 0\,, \tag{2.9}$$

an assumption motivated by the structure of physical models. The key property (2.9) and physically grounded structural hypotheses (imposed in [31]) provide a strong stabilization mechanism for the relaxation models (2.8). It must be highlighted that the construction of the relaxation system (2.8) together with (2.9) requires significant effort (but depending directly on the structure of the equations in (2.7)).

My Contribution. The main contribution of the article [31] can be characterized as follows: (a) The novel framework extends the theory of A. Tzavaras [55] (for hyperbolic conservation laws) to *inhomogeneous* hyperbolic balance laws. It provides a rigorous proof of the relaxation limit with a

convergence rate of order $\mathcal{O}(\varepsilon)$ for a large class of physically relevant systems of hyperbolic balance laws. The analysis treats a large class of source terms: those satisfying a special mechanism that induces *weak dissipation* [11], which means that $[\mathrm{D}H(U) - \mathrm{D}H(M(V)][G(U) - G(V))] \leq 0$, as well as a more general source term. (b) The work [31] describes how, given a certain physical system governed by a hyperbolic balance law, one can construct a relaxation approximation system endowed with a globally defined, convex entropy $H(U)$. The analysis treats a large class of physical systems such as the system of elasticity, two phase flow models, and general symmetric hyperbolic systems.

2.3.2 Relaxation models for balance laws via a wave operator [32]

The convergence properties of relaxation systems and associated relaxation schemes for scalar conservation laws are presently well understood (see [3, 9, 21, 35]). By contrast, the relaxation approximation of inhomogeneous systems of hyperbolic balance laws presents major additional challenges and it is the subject of current intense research investigation.

In the work [32] K. Trivisa and I introduced a class of relaxation models for the approximation of solutions to the hyperbolic balance law

$$\partial_t u + \sum_{j=1}^{d} \partial_{x_j} F_j(u) = G(u)\,, \quad u \in \mathbb{R}^n,\, (x,t) \in \mathbb{R}^d \times \mathbb{R}_+ \tag{2.10}$$

(equipped with the entropy-entropy flux pair η-q) and addressed the issues of stability and convergence. The class of relaxation schemes introduced in this work are of the form

$$\partial_t u + \sum_{j=1}^{d} \partial_{x_j} v_j = 0\,, \quad \partial_t v_i + A_i \partial_{x_i} u = -\frac{1}{\varepsilon}\Big(v_i - F_i(u) + \mathcal{R}_i[u](x,t)\Big) \quad i = 1, \dots, d\,, \tag{2.11}$$

with $v_i \in \mathbb{R}^n$, A_i symmetric, positive definite matrix, and the global term

$$\mathcal{R}_i[u](x,t) = \frac{1}{d} \int^{x_i} G(u(x_1, \dots, x_{i-1}, z, x_{i+1}, \dots, x_d, t))\, dz. \tag{2.12}$$

The approximations (2.11) are based on the relaxation models of Jin and Xin [21] for hyperbolic conservation laws without source terms. The stabilization mechanism in the models (2.11)-(2.12) (as well as those in [21]) is the regularization by the *wave operator* $\big(\sum_{j=1}^{d} A_j u_{x_j x_j} - u_{tt}\big)$, which explicitly appears when v_i is excluded from $(2.11)_1$.

My Contribution. The novel class of relaxation models (2.11) introduced in my work is suitable for the approximation of solutions to a vast array of *inhomogeneous* systems of hyperbolic balance laws (arising in continuum physics) with a source term G satisfying a special mechanism that induces weak dissipation [11] as well as a more general source term. There are two main novelties in my work: (a) In the introduction of the global term $\mathcal{R}_i[u]$ in the relaxation models (2.11)-(2.12); and (b) In the extension of the relative entropy method (used to establish convergence) to the relaxation models (2.11). The *modified relative entropy method* presented in my work relies on a *relative potential* associated with the term $\mathcal{R}_i[u]$. The introduction of this concept was required in order to deal with the weakly dissipative source term G which typically satisfies no growth conditions. The relative potential assists in "tracking" the contribution of the (weakly dissipative) source term G; it becomes a part of a Lyapunov functional which monitors the evolution of the difference between the relaxation and equilibrium solutions and provides a convergence rate of order $\mathcal{O}(\varepsilon^2)$ before the formation of shocks.

3 Current Research

My research at the University of Massachusetts Amherst focuses on the development of numerical methods for systems of multidimensional hyperbolic conservation laws that are based on the relaxation models and variational methods developed in my previous works [28, 29, 17, 30, 31, 32]. I am also involved in several projects relevant to mathematical biology [46, 19] and statistics [33].

3.1 Finite element schemes for three-dimensional elastodynamics [34]

The elasticity system (2.1), recast as a system of conservation laws,

$$\partial_t F_{i\alpha} = \partial_\alpha v_i\,, \quad \partial_t v_i = \partial_\alpha\Big(\frac{\partial W}{\partial F_{i\alpha}}(F)\Big)\,, \tag{3.1}$$

comprises of twelve highly nonlinear equations and therefore the only way to compute practical solutions is to compute them numerically. Moreover, solutions to elastodynamics admit solutions that exhibit shocks (discontinuities), cavitating solutions and non-uniqueness of solutions [1, 7, 30, 42]. These issues present both computational and theoretical challenges for the design of numerical methods used to approximate solutions.

In the joint work [34] with N. Walkington (Carnegie Mellon University) I am developing a fully-discrete numerical scheme and computer code for computing solutions to three-dimensional polyconvex elastodynamics (2.1) that is discrete in both time and space with the aim to test the numerical method on real-life applications using computer simulations.

The scheme is based on the innovative *time-discrete* variational approximation method of [13] used to approximate solutions to elasticity equations with polyconvex stored energy, energy of the form $W(F) = G(F, \operatorname{cof} F, \det F) = G \circ \Psi(F)$; the method in [13] is used to construct the sequence of iterates $\{v^n \in \mathbb{R}^3, \Xi^n \in \mathbb{R}^{19}\}_{n\geq 1}$ that solve equations (2.2), the time-discretized version of the extended elasticity system (see Section 1.1.1).

The main challenge in the current work is to adapt the minimization framework of [13] to space-discrete settings, which can be accomplished by an appropriately designed finite element method. Motivated by the time-discrete scheme (2.2) I propose the following numerical method: given appropriate finite element spaces U_h, H_h, and data $(v_h^{n-1}, \Xi_h^{n-1}) \in U_h \times H_h$ at time step $t = t_{n-1}$ construct the next iterate by solving

$$\begin{aligned} \tfrac{1}{\Delta t}\big(v_h^n - v_h^{n-1}, \varphi_h\big) &= -\big(D_\Xi G(\Xi_h^n), D_F\Psi(F_h^{n-1})\nabla\varphi_h\big) && \forall \varphi_h \in U_h \\ \tfrac{1}{\Delta t}\big(\Xi_h^n - \Xi_h^{n-1}, \psi_h\big) &= \big(D_F\Psi(F_h^{n-1})\nabla v^n, \psi_h\big) && \forall \psi_h \in H_h\,. \end{aligned} \tag{3.2}$$

To realize the finite element scheme (3.2) it is essential to identify appropriate finite element spaces used in space discretization as well as establish the convergence and provide an error estimate for the approximation. In the preliminary work [34] N. Walkington and I identified suitable finite element spaces that render the finite element scheme *dissipative* and *unconditionally stable*, which are necessary requirements for any reliable numerical method. Our analysis follows in spirit the analysis presented in [29] where I established the direct convergence of iterates produced by the time-discrete scheme (2.2) (for details see Section 1.1.1). In particular, we consider the relative entropy

$$\eta^r = \tfrac{1}{2}|V^{(\Delta t,h)} - \bar{V}|^2 + \big[G(\Xi^{(\Delta t,h)}) - G(\bar{\Xi}) - D_\Xi G(\bar{\Xi})(\Xi^{(\Delta t,h)} - \bar{\Xi})\big]$$

that estimates the difference between approximations $V^{(\Delta t,h)}, \Xi^{(\Delta t,h)}$ generated by the numerical scheme and the solution $(\bar{V}, \bar{\Xi})$ of the extended elasticity system and derive *the relative entropy identity* that monitors the time evolution of η^r. The relative entropy identity is central to establishing the convergence and providing an error estimate. At the moment our research efforts are focused on the estimation of the terms in the relative entropy identity as well as on the implementation of the finite element scheme in a computer code and developing suitable benchmark problems for testing the scheme numerically.

3.2 Finite element relaxation schemes via a wave operator

The problem of numerical approximation of hyperbolic balance laws is a challenging one due to the presence of shocks that propagate in time. Such methods need to resolve accurately the shock regions and at the same time approximate with high accuracy the regions where the solution is smooth. The presence of source terms that appear in many hyperbolic systems arising in continuum physics presents a number of additional challenges and requires a delicate treatment.

In the joint project with K. Trivisa (University of Maryland, College Park) I am developing finite element schemes for the approximation of solutions to the hyperbolic balance law,

$$\partial_t u + \sum_{j=1}^{d} \partial_{x_j} F_j(u) = G(u), \quad u \in \mathbb{R}^n,\ (x,t) \in \mathbb{R}^d \times \mathbb{R}_+ ,$$

equipped with the entropy identity (which is the case for many systems arising in continuum physics [12]) with source terms satisfying a special mechanism that induces dissipation in the spirit of Dafermos [11] as well as more general source terms.

The proposed finite element schemes are based on the relaxation models (2.11) introduced in my previous work [32] (see Section 1.3.2). The class of fully-discrete finite element schemes is as follows: given the m-th time iterates $\big(u^m, v_1^m, \dots, v_d^m\big) \in S_k \times V_{k-1}^d$, with S_k, V_{k-1} appropriate finite element spaces, the $(m+1)$-st iterates are constructed by solving the explicit system

$$\begin{aligned} &\tfrac{1}{h}\big(u^{m+1} - u^m, \varphi\big) - \sum_{i=1}^{d} \big(v_i^n, \partial_{x_i}\varphi\big) = 0 \\ &\tfrac{1}{h}\big(v_i^{m+1} - v_i^m, \psi\big) + \big(A_i\, \partial_{x_i} u^{m+1}, \psi\big) = -\tfrac{1}{\varepsilon}\big(v_i^{m+1} - F_i(u^{m+1}) + \mathcal{R}_i[u^{m+1}],\, \psi\big). \end{aligned} \tag{3.3}$$

for all $\varphi \in S_k,\ \psi \in V_{k-1}$, where $\mathcal{R}_i$ (the novel feature of the relaxation models (2.11) introduced in [32]) is a global term defined in (2.12). The finite-element scheme (3.3) is motivated by the work of Arvanitis, Makridakis and Tzavaras [2] for systems of hyperbolic conservation laws without source terms.

At the moment our research efforts are focused on establishing the stability of the scheme (3.3) and deriving the rate of convergence (using the modified relative entropy of [32] method adapted to the subject of finite element discretization). The scheme (3.3) has been implemented in computer code and is in the testing process. In addition, to avoid oscillatory behavior near the shock, I am reinforcing the current implementation with adaptive mesh refinement following the ideas in [2, 4].

3.3 Projects in Mathematical Biology

At certain point in my postdoctoral life I decided that at least some part of my work must have a broader impact on the scientific community. I felt the need to participate in applied projects and interact with people from different disciplines in order to learn about other subjects. This urge resulted in my participation in several applied projects, two of which are relevant to modelling of biological systems. The first work [46] (which is more on the applied side) is a joint project with a microbiologist J. Philips (University of Leuven, Belgium and University of Massachusetts, Amherst) and her collaborators. In this work the migration of *Geobacter* bacteria is studied experimentally and via modelling. In the second work, a joint project with P.-E. Jabin (University of Maryland, College Park), I am studying a *cooperation* phenomena in structured biological populations by the example of bacteria degrading cellulose. Below are some of the details.

3.3.1 Migration of *Geobacter* bacteria [46]

The chemical trichloroethene (TCE) is a widespread groundwater pollutant. Remediation of soils contaminated with this chemical is challenging because TCE accumulates deep in subsurface as a

separate liquid, i.e. a dense non-aqueous phase liquid (DNAPL). The use of bacteria that degrade TCE offers perspectives to clean up such contaminations. Biodegradation in a contaminated subsoil can be slow; in such cases, bioaugmentation (the injection of TCE degrading microbial culture) can initiate the clean-up process (see [5, 8, 57]). The subsoil zones containing DNAPL are hard to reach if bacterial transport relies only on the groundwater flow. Thus microbial migration, which can be due to random motility (swimming of the bacteria in random directions) or chemotaxis (bacterial swimming towards or away from a chemical gradient), towards a DNAPL could greatly accelerate bioaugmentation (see [15, 49, 50]). Until now, however, it remained unknown whether TCE degrading bacteria are able to migrate towards a TCE DNAPL and can initiate the clean-up process. Motility had been reported for *Geobacter* lovleyi SZ [16], which is interesting since this species is often used for the bioaugmentation of TCE contaminated subsoils. The objective of the current collaborative project [46] (by J. Philips, A. Miroshnikov, P. J. Haest, D. Springael and E. Smolders) is to investigate the motility and potential chemotaxis of *Geobacter* and to examine the effect of their migrational properties on the degradation of a TCE DNAPL.

Diffusion-cell experiment and modelling. J. Philips conducted various experiments using a TCE degrading culture similar to *Geobacter* lovleyi SZ. Specifically, she conducted chemotaxis assays (and found no evidence for it) as well as experiments in which the effect of the motility of the *Geobacter* bacteria on the degradation of a TCE DNAPL was investigated. The effect of the motility was studied using a three-layer diffusion-cell setup [44]. This setup uses a glass cylinder in which 3 layers are created: a bottom 3.5 cm TCE DNAPL layer, a central 5.5 cm sand layer, and an upper 3 cm aqueous layer. The top layer was frequently refreshed to act as a zero-sink for TCE. The *Geobacter* bacteria were added to the top layer and their migration through the sand layer and concurrent degradation of TCE was measured.

To clarify how the motility of *Geobacter* contributed to the observed TCE degradation in the diffusion-cell experiment a diffusion-motility model was developed. The initial model used by J. Philips used oversimplified boundary conditions, and therefore produced results that did not agree with the experimental outcome. The original model dealt with the sand layer only, without taking into account that bacteria can migrate in between layers (one of which was frequently refreshed). I redesigned the model to reflect the physical properties of the diffusion-cell setup. We use a reaction-diffusion system of the form

$$\begin{aligned} \partial_t C_i(t,z) &= \partial_z\Big(D_i(z)\partial_z C_i(t,z)\Big) + f_{GEO}(C_i, z; q) \\ z \in I_i,\ \ C_i \in \mathbb{R}^3,\ \ i &= 1,2,3\,,\ \ q \in \mathbb{R}^8\,, \end{aligned} \tag{3.4}$$

subject to the *interface* conditions for the fluxes,

$$J_{12}^-(t) = J_{12}^+(t)\,, \quad J_{23}^-(t) = J_{23}^+(t)\,, \tag{3.5}$$

between the adjacent layers I_1-I_2 and I_2-I_3, respectively. Here I_i is the interval representing the i-th zone: $I_1 = [-3.5, 0]$ is the DNAPL layer, $I_2 = [0, 5.5]$ sand layer and $I_3 = [5.5, 8.5]$ is aqueous layer (refreshed twice a week). The vector $C^i = (C_{i1}, C_{i2}, C_{i3})$ corresponds to concentrations of TCE, *Geobacter* and the degradation product cis-dichloroethene (DCE) in the i-th zone, respectively, and $J_{12}^{\pm}$ and $J_{23}^{\pm}$ denote the fluxes between layers. Incorporation of the flux conditions (3.5) into the model allows me to take into account the migration of bacteria between layers and effects the overall biodegradation dynamics. The term f_{GEO} (designed in accordance with experiments conducted by J. Philips) encodes the growth behaviour of *Geobacter* and their TCE degradation rate.

I implemented the new model (3.4) in a computer code and conducted various numerical experiments the results of which are used in the paper [46]. In addition, I investigated the sensitivity of the model towards its various parameters $q \in \mathbb{R}^8$ (incorporated in the source term f_{GEO}) using Morris' one-at-a-time sensitivity analysis (see [27]).

3.3.2 Cooperation phenomena in structured biological populations [19]

In the joint work [19] with P.-E. Jabin I study the evolutionary dynamics in biological populations structured by a parameter describing a biological, physiological or ecological characteristic of the individuals (such characteristic is called a *trait* [43]). The aim of the present work is to study *cooperation* among the individuals in certain biological populations (roughly speaking, such phenomena are reflected by a population growth rate which is super-linear with respect to the population size). Typical models describing the population dynamics take only competition into account neglecting the fact that for relatively small populations cooperation may play an important role (as, for instance, small populations may survive for longer periods of time).

In the present work I am developing models describing *cellulose biodegradation* processes (in which cooperation may potentially be present) and study multiple-trait populations as well as investigate continuous-trait models that appear in the limit. The mechanisms that initiate cooperation in these models have been discussed extensively with a microbiologist J. Phillips (University of Leuven, Belgium and University of Massachusetts, Amherst).

Cellulose Biodegradation. Cellulose is the structural component of many plants and is therefore the most abundantly produced biopolymer; it is a homopolymer consisting of vast number of glucose units. The most important feature of cellulose as a substrate is its *insolubility*. As such, bacterial and fungal degradation of cellulose occurs exocellularly (e.g. by fungi *Trichoderma reesei* or bacteria *Clostridium thermocellum*). The products of cellulose hydrolysis are available as carbon and energy sources for microbes that inhabit environments in which cellulose is biodegraded [23, 26].

Mechanisms and Models. The cellulose biodegradation in our work is modeled as the multiple-step process described as follows. Let $n(t) = \sum_j n_j(t)$ denote the biomass density of a certain microorganism that degrades cellulose, with $n_j(t)$ the biomass density of individuals with a trait x_j, $j \in \{1, \dots, M_n\}$. Here the parameter x_j is a certain characteristic of the microorganism (for instance, x_j may encode the ability to convert product of degradation into energy or reflect the structure, such as size, of the microorganism). Let $\varrho_i(t)$ denote a mass of cellulose with a structural parameter i, with $i \in \{1 \dots M_\varrho\}$ (the parameter i may correspond to the crystallinity of the cellulose, the number of cellobiose units in the cellulose or the number of reducing and nonreducing ends).

The biodegrading microorganism is unable to consume (degrade) the cellulose directly. Instead, the individuals, with a trait x_j, produce two enzyme complexes $e_{1,j}(t)$ and $e_{2,j}(t)$ that act in a sequential order. During the first stage the (endoglucanase) enzyme $e_{1,j}$ weakens cellulose fibers, that is, it randomly cuts the fibers by creating the so called reducing and nonreducing ends serving as landing sites for the (exoglucanase) enzyme $e_{2,j}$. During the second stage the enzyme $e_{2,j}$ locates a reducing (or a nonreducing) end and then attaches itself to it. Once attached it cleaves off cellobiose (a major energy source for the microorganisms) off the chain of polysaccharide. Some portion $\theta_p \in [0, 1]$ of cellobiose is consumed directly by the microorganism that produced the enzymes and the rest is available for other individual microorganism in the population due to diffusion.

In our work P.-E. Jabin and I developed several models that differ in complexity. Even in the simplest model (corresponding to $M_n = M_\varrho = 1$) the aforementioned cascade of events inadvertently produces *cooperation* (which appears in view of the fact that the cellobiose units cleaved off by the enzyme of one microorganism are available for consumption by another individual located nearby). Mathematically, these effects are encoded in the growth rate $B(n)$ of the population n. In particular, for small populations the population size $n(t)$ turns out to behave as

$$\partial_t n(t, \cdot) \sim n\big(B(n) - d\big) \quad \text{with} \quad B(n) \sim Cn^2 \quad \text{for} \quad n << 1.$$

At the moment I am focusing on the studies of cooperation in more complex models for multiple-trait populations as well as continuous-trait model generated in the limit as $\Delta x = x_j - x_{j-1} \to 0$ and $M \to \infty$. I expect that the mathematical models developed in the present work will produce

better phenomenological results for small populations when cooperation significantly effects the dynamics.

3.4 `parallelMCMCcombine`: An R Package for Bayesian Methods for Big Data and Analytics (computational statistics) [33]

In this age of big data and analytics, statisticians are facing new challenges due to the exponential growth of information being produced. Here, big data refers to data sets that are too large and complex for classic analysis tools to be used. An extensive number of application areas are affected by big data, including genomics, healthcare, energy, finance, sustainability and meteorology. One primary difficulty in analyzing these large data sets is the restriction on file sizes that can be read into computer memory; in addition, it may be necessary to store and process data sets on more than one machine due to their large sizes. Several recent Bayesian and Markov chain Monte Carlo (MCMC) methods have been developed to address these issues, where data sets are large only due to large sample sizes. One approach partitions large data sets into smaller subsets, and parallelizes the MCMC computation by analyzing the subsets on separate machines (Langford [22], Newman [38], Smola [52]); here, information is exchanged at each iteration of the Markov chains, requiring communication between machines. Due to the slow performance of these techniques, alternative methods have been introduced that do not require communication between machines (Neiswanger [37], Scott [48]). These recent methods divide the data into subsets, perform Bayesian MCMC computation on the subsets, and then combine the results back together; the separate analyses are run independently, and are thus parallel, communication-free methods. Specifically, Neiswanger [37] introduces several kernel density estimators that approximate the posterior density for each data subset; the full data posterior is then estimated by multiplying the subset posterior densities together. Alternatively, Scott [48] developed methods that combine subset posteriors into the approximated full data posterior using weighted averages over the subset MCMC samples.

The subset-based parallel communication-free MCMC methods hold great promise for the future of Bayesian big data analysis and analytics research. In the joint work [33] E. Conlon (University of Massachusetts Amherst) and I introduce the R package `parallelMCMCcombine` for implementing four of these methods, including those of Neiswanger [37] and Scott [48]; in [33] we introduce each of the four methods, describe the main functions and features of the package, and demonstrate the package using both simulated and real data sets. The package assumes that the user has produced the independent subposterior MCMC samples by carrying out the Bayesian analysis outside of the R-package, either within R or in a separate software package such as WinBUGS [25], JAGS [20], or Stan[53, 54]; the user then reads the results into our R package. The methods are best suited to models with unknown parameters of fixed dimension in continuous parameter spaces (see [37, 48]). The `parallelMCMCcombine` package is implemented in R (R Development Core Team 2014) and is available from the Comprehensive R Archive Network at `http://CRAN.R-project.org`.

4 Future Research Plans

In the future I plan to explore new research directions as well as develop further the ideas discussed in my past works. Specifically, I will continue investigating problems that arise in mechanics and continuum physics (cavitation, hyperbolic conservation laws, nonlinear elastodynamics, relaxation approximation models, etc.) and continue learning and working in the area of mathematical biology (models relevant to cell population dynamics, motion of ciliated and flagellated organisms). Also, I intend to work on challenging and exciting problems relevant to big data analysis and analytics research (in the statistical context). Finally, I plan to participate in the projects relevant to inverse problems and uncertainty quantification analysis; these problems are appealing to me as they lie in the intersection of several disciplines: partial differential equations, probability, statistics and computer science. Below are the details of some of my plans.

Modeling of ciliated and flagellated organisms. In August 2014 I participated in IdeaLab2014, a program for young researchers at ICERM, Brown University. The aim of the program was to develop new, more realistic models of ciliated and flagellated organisms. In the course of the program my collaborators Cristi Guevara (Louisiana State University) and Will Cousins (Massachusetts Institute of Technology) and I developed a novel modeling approach relevant to cilia motion (for both an individual cilia as well as a group of interacting cilia). In the future I plan to develop the ideas generated during the programm further with the main objective to design computer models that capture cilia motions more realistically.

Mechanics. Little is known at present concerning (existence and uniqueness for) solutions to the radial elasticity system (2.3). I worked with the radial elasticity system previously (see [28, 29]) and plan to continue studying these fascinating, but difficult equations. In the joint project Robin Young (University of Massachusetts Amherst) and I developed an approach that allows us to study radial solutions $y(x,t) = w(R,t)\frac{x}{R}$ to elastodynamics (2.1) by means of relaxation models. The relaxation models [21, 32] (employing the wave operator) might be adopted to approximate the radial elasticity equations by transforming the relaxation system (in the form (2.11)) that approximates the equations of elasticity (2.1) into the system whose solutions are radial. The preliminary energy estimates of the radial relaxation system, however, indicate that there is not enough dissipation (coming from relaxation) to provide stability of its solutions. This motivated us to seek for an alternative relaxation system. We consider a more general class of solutions to the equations of elasticity (2.1). These have the form $y(x,t) = Q(R,t)w(R,t)\frac{x}{R}$, with $R = |x|$ and $Q(R,t) \in SO(3)$ is a proper rotation; we call them *radial whirling* solutions. The class of such solutions includes radial ones but is much wider. In the future I would like to derive and study the equations for whirling radial solutions and (based on these equations) construct the corresponding relaxation models that can be used to study solutions of radial equations (2.3). I believe that such relaxation systems may possess enough dissipation to provide stability. In addition, the family of whirling solutions is very rich, it contains solutions with both shock and rarefaction waves, and I plan to investigate wave interactions within the class of radial whirling solutions following in the spirit the analysis of Robin Young [58, 59] for elastic strings in three dimensions.

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