Stability of fully discrete variational schemes for elastodynamics with a polyconvex stored energy

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Abstract

In this article we develop a fully discrete variational scheme that approximates the equations of three dimensional elastodynamics with polyconvex stored energy. The fully discrete scheme is based on a time-discrete variational scheme developed by S. Demoulini, D. M. A. Stuart and A. E. Tzavaras (2001). We show that the fully discrete scheme is unconditionally stable. The proof of stability is based on a relative entropy estimation for the fully discrete approximates.

1 Introduction

The equations describing the evolution of a continuous medium with nonlinear elastic response and zero body forces in referential description are given by

\[
\frac{\partial^2 y}{\partial t^2} = \text{div} S(\nabla y) \tag{1.1}
\]

where \( y(x,t) : \Omega \times [0,\infty) \rightarrow \mathbb{R}^3 \) stands for the elastic motion, \( S \) for the Piola-Kirchhoff stress tensor and the region \( \Omega \) is the reference configuration of the elastic body.

The equations (1.1) are often recast as a system of conservation laws,

\[
\begin{align*}
\partial_t v_i &= \partial_{x_\alpha} S_{\alpha i}(F) \\
\partial_t F_{i\alpha} &= \partial_{x_\alpha} v_i,
\end{align*} \tag{1.2}
\]

for the velocity \( v = \partial_t y \in \mathbb{R}^3 \) and the deformation gradient \( F = \nabla y \in M_{3 \times 3} \) and we use the summation convention over repeated indices. The differential constraints

\[
\partial_\beta F_{i\alpha} - \partial_\alpha F_{i\beta} = 0 \tag{1.3}
\]

are propagated from the kinematic equation (1.2) and are an involution [7].

For hyperelastic materials the first Piola-Kirchhoff stress tensor \( S(F) = \frac{\partial W}{\partial F}(F) \) is expressed as the gradient of the stored-energy function of the elastic body

\[
W(F) : M_{3 \times 3}^+ \rightarrow \mathbb{R}^3 \quad \text{where} \quad M_{3 \times 3}^+ := \{ F \in M_{3 \times 3} : \det F > 0 \}. \tag{1.4}
\]

Convexity of the stored energy is, in general, incompatible with certain physical requirements and is not a natural assumption. As an alternative, we consider polyconvex stored energy \( W \), which means that

\[
W(F) = G(F, \text{cof } F, \det F) = G \circ \Phi(F), \quad \Phi(F) = (F, \text{cof } F, \det F) \tag{1.4}
\]

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where
\[ G = G(\xi) = G(F, Z, w) : M^3_{13} \times M_{33} \times \mathbb{R} \cong \mathbb{R}^{19} \rightarrow \mathbb{R} \] (1.5)
is a convex function.

For polyconvex stored energies \[ (1.4) \] the system of elasticity \[ (1.1) \] is expressed by
\[
\partial_t v_i = \partial_{x_a} \left( \frac{\partial G}{\partial \xi_a}(\Phi(F)) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \right),
\]
\[
\partial_t F_{i\alpha} = \partial_{x_a} v_i
\] (1.6)
which is equivalent to \[ (1.1) \] subject to differential constraints \[ (1.3) \] that are an involution \[ (7) \]: if they are satisfied for \( t = 0 \) then \[ (1.3) \] propagates \[ (1.3) \] to satisfy for all times. Thus the system \[ (1.6) \] is equivalent to systems \[ (1.1) \] whenever \( F(\cdot, 0) \) is a gradient. Most importantly the system \[ (1.6) \] is endowed with the entropy identity
\[
\partial_t \left( \frac{|v|^2}{2} + G(\Phi(F)) \right) - \partial_{x_a} \left( v_i \frac{\partial G}{\partial \xi_a}(\Phi(F)) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \right) = 0.
\] (1.7)

In the present work we are concerned with the design of a numerical method along with a numerical analysis theory for solutions to the equations of elastodynamics with polyconvex stored energies. The main objective of this work is to develop fully-discrete numerical scheme for equation \[ (1.6) \] based on the time-discrete variational method introduced by Stuart, Demoulini and Tzavaras \[ (11) \]. The variational method in \[ (11) \] is used to approximate solutions of elasticity equations with polyconvex stored energy. In \[ (11) \] the equations \[ (1.6) \] are embedded into a larger system
\[
\partial_t v_i = \partial_{x_a} \left( \frac{\partial G}{\partial \xi_a}(\xi) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) \right),
\]
\[
\partial_t \xi_A = \partial_a \left( \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) v_i \right)
\] (1.8)
that has variables \( v \in \mathbb{R}^3, \xi \in \mathbb{R}^{19} \) and is equipped with a convex entropy \( \eta(v, \xi) = \frac{1}{2} |v|^2 + G(\xi) \).

The convexity of the entropy \( \eta \) allows the authors to employ variational techniques in time-discrete settings. The variational method produces the sequence of spatial iterates \( \{v^n, \xi^n\}_{n \geq 1} \) that solve the time-discretized version of the enlarged elasticity system,
\[
\frac{1}{\Delta t}(v_i^n - v_i^{n-1}) = \partial_a \left( \frac{\partial G}{\partial \xi_a}(\xi^n) \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^{n-1}) \right) \quad \text{in} \quad \mathcal{D}'(\mathbb{T}^3),
\]
\[
\frac{1}{\Delta t}(\xi_A^n - \xi_A^{n-1}) = \partial_a \left( \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F^{n-1}) v_i^n \right)
\] (1.9)
and give rise to time-continuous approximates converging to the solution of elastodynamics before shock formation (see \[ (15) \]).

The main challenge in the present work is to adapt the minimization framework of \[ (11) \] to space-discrete settings, which can be accomplished by an appropriately designed finite element method. To realize the finite element scheme it is essential a) to identify appropriate finite element spaces used in space discretization, b) to provide an error estimate for the approximation, and c) to test the finite element scheme numerically.

In our present work we introduce the following numerical method: given appropriate finite element spaces \( U_h, H_h, \) and data \( \{v_i^{n-1}, \xi_A^{n-1}\} \in U_h \times H_h \) at time step \( t = t_{n-1} \) construct the next iterate by solving
\[
\frac{1}{\Delta t}(v_i^n - v_i^{n-1}, \varphi_h) = -\langle D\xi G(\xi_h^n), D_F\Phi(F_h^{n-1})\nabla \varphi_h \rangle, \quad \forall \varphi_h \in U_h
\]
where \( \xi_h^n = \xi_h^{n-1} + \Delta t (D_F\Phi(F_h^{n-1})\nabla v^n) \in H_h \).
\] (1.10)
In this work we introduce suitable finite element spaces that render the finite element scheme \( 1.10 \) unconditionally stable, which is a necessary requirement for any reliable numerical method. The spaces of test functions are rich enough that an important (gradient) conservation property

\[
\Delta t F^j_h - F^{j-1}_h = \nabla v^j_h \quad \text{is satisfied by the finite element approximation at each time step. This property is essential in adapting the method of [11] to a fully discrete scheme. The existence of numerical solutions to \( 1.10 \) is obtained using minimization principles.}
\]

In this article we establish the stability of numerical solutions and derive the relative entropy identity which is central to establishing the convergence and providing an error estimate. Our stability analysis follows in spirit the work of Miroshnikov and Tzavaras [15] where the authors established the direct convergence of iterates produced by the time-discrete scheme \( 1.9 \).

Specifically, following [15], we consider the relative entropy

\[
\eta^r = \frac{1}{2} |V^{(\Delta t,h)}(x,t) - \overline{V}(x,t) - D \Xi G(\overline{\Xi}(\Delta t,h)) - \overline{G}(\Xi(\Delta t,h) - \Xi)|^2
\]

that estimates the difference between time-continuous approximations \( V^{(\Delta t,h)}(x,t) \) and \( \overline{V}(x,t) \), the classical solution \( \Xi(\Delta t,h) \) of the extended elasticity system and derive the relative entropy identity

\[
\int_{\Omega} \left\{ \partial_t \eta^r(x,t) + \partial_{x_\alpha} q^\alpha_\alpha(x,t) \right\} dx = \int_{\Omega} \left( -\frac{1}{\Delta t} D + Q + E \right) dx \quad (1.11)
\]

that monitors the time evolution of \( \eta^r \). Here \( D > 0 \) is the dissipation produced by the scheme, \( Q \) is the term equivalent to \( \eta^r \), and \( E \) is the error term. The relative entropy identity is central to establishing the stability of the scheme and providing an error estimate; establishing the convergence of the approximates is the subject of future investigations.

2 Time-discrete variational approximation scheme

2.1 Time-discrete scheme and its stability

In this section we briefly describe the semi-discrete variational scheme of Demoulini, Stuart and Tzavaras [11] as well as the result of the article [15] in which to avoid inessential difficulties the authors work with periodic boundary conditions, i.e., the spatial domain \( \Omega = \mathbb{T}^3 \) is taken to be the three-dimensional torus.

The work [11] uses extensively the properties of so-called null-Lagrangians. To this end we recall its definition:

**Definition 2.1.** A continuous function \( L(F) : M^{3 \times 3} \rightarrow \mathbb{R} \) is a null-Lagrangian if

\[
\int_{\Omega} L(\nabla (u + \varphi)) \, dx = \int_{\Omega} L(\nabla u) \, dx \quad (2.1)
\]

for every bounded open set \( \Omega \subset \mathbb{R}^3 \) and for all \( u \in C^1(\overline{\Omega}; \mathbb{R}^3) \), \( \varphi \in C^\infty_0(\Omega; \mathbb{R}^3) \).

It turns out that the components of \( \Phi(F) \) defined in (1.4) are null-Lagrangians and satisfy

\[
\partial_{\alpha} \left( \frac{\partial \Phi^A}{\partial F_{i\alpha}}(\nabla u) \right) = 0, \quad A = 1, \ldots, 19 \quad (2.2)
\]

for any smooth \( u(x) : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \). Therefore, for smooth solutions \( (v, F) \) of (1.6), the null-Lagrangians \( \Phi^A(F) \) satisfy the transport identities [10]

\[
\partial_t \Phi^A(F) = \partial_{\alpha} \left( \frac{\partial \Phi^A}{\partial F_{i\alpha}}(F) v_i \right), \quad \forall F \quad \text{with} \quad \partial_\beta F_{i\alpha} = \partial_{i\alpha} F_{\beta}. \quad (2.3)
\]
Due to the identities (2.3) the system of polyconvex elastodynamics (1.6) can be embedded into the enlarged system [10]

\[
\begin{align*}
\partial_t v_i &= \partial_\alpha \left( \frac{\partial G}{\partial \xi_A} (\xi) \frac{\partial \Phi^A}{\partial F_{\alpha i}} (F) \right) \\
\partial_t \Phi_A &= \partial_\alpha \left( \frac{\partial \Phi^A}{\partial F_{\alpha i}} (F) v_i \right)
\end{align*}
\] (2.4)

The extension has the following properties:

(E1) If \( F(\cdot, 0) \) is a gradient then \( F(\cdot, t) \) remains a gradient \( \forall t \).

(E2) If \( F(\cdot, 0) \) is a gradient and \( \xi(\cdot, 0) = \xi(F(\cdot, 0)) \), then \( F(\cdot, t) \) remains a gradient and \( \xi(\cdot, t) = \xi(F(\cdot, t)) \), \( \forall t \). In other words, the system of polyconvex elastodynamics can be viewed as a constrained evolution of (2.4).

(E3) The enlarged system admits a convex entropy

\[
\eta(v, \xi) = \frac{1}{2} |v|^2 + G(\xi), \quad (v, \xi) \in \mathbb{R}^{22}
\] (2.5)

and thus is symmetrizable (along the solutions that are gradients).

Based on the time-discretization of the enlarged system (2.3) S. Demoulini, D. M. A. Stuart and A. E. Tzavaras [10] developed a variational approximation scheme which, for the given initial data

\[
\Theta^0 := (v^0, \xi^0) = (v^0, F^0, Z^0, w^0) \in L^2 \times L^p \times L^2 \times L^2
\] (2.6)

and fixed time step \( \tau > 0 \), constructs the sequence of successive iterates

\[
\Theta^n := (v^n, \xi^n) = (v^n, F^n, Z^n, w^n) \in L^2 \times L^p \times L^2 \times L^2, \quad n \geq 1
\] (2.7)

with the following properties (see [11] Lemma 1, Corollary 2):

(P1) The iterate \((v^n, \xi^n)\) is the unique minimizer of the functional

\[
\mathcal{J}[v, \xi] = \int_{T^3} \left( \frac{1}{2} |v - v^{n-1}|^2 + G(\xi) \right) dx
\]

over the weakly closed affine subspace

\[
\mathcal{C} = \left\{ (v, \xi) \in L^2 \times L^p \times L^2 \times L^2 : \text{such that } \forall \varphi \in C^\infty(T^3) \right. \\
\left. \int_{T^3} \left( \frac{\xi_A - \xi_A^{n-1}}{\tau} \right) \varphi dx = - \int_{T^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha i}} (F^{n-1}) \right) v_i \partial_\alpha \varphi dx \right\}.
\]

(P2) For each \( n \geq 1 \) the iterates satisfy the corresponding Euler-Lagrange equations

\[
\begin{align*}
\frac{v^n_i - v^{n-1}_i}{\tau} &= \partial_\alpha \left( \frac{\partial G}{\partial \xi_A} (\xi^n) \frac{\partial \Phi^A}{\partial F_{\alpha i}} (F^{n-1}) \right) \\
\frac{\xi_A^n - \xi_A^{n-1}}{\tau} &= \partial_\alpha \left( \frac{\partial \Phi^A}{\partial F_{\alpha i}} (F^{n-1}) v_i^n \right)
\end{align*}
\] (2.8)

(P3) If \( F^0 \) is a gradient, then so is \( F^n \), \( \forall n \geq 1 \).

(P4) Iterates \( v^n, n \geq 1 \) have higher regularity: \( v^n \in W^{1,p}(T^3), \forall n \geq 1 \).

(P5) There exists \( E_0 > 0 \) determined by the initial data such that

\[
\sup_{n \geq 0} \left( \|v^n\|_{L^2_x}^2 + \int_{T^3} G(\xi^n) \right) dx + \sum_{n=1}^{\infty} \|\Theta^n - \Theta^{n-1}\|_{L^2_x}^2 \leq E_0.
\] (2.9)
2.2 Convergence of the time-discrete scheme

In [15] we established the direct convergence of time-continuous interpolates,

\[
\hat{v}^{(\tau)}(t) = \sum_{n=1}^{\infty} X^n(t) \left( v^{n-1} + \frac{t - \tau(n-1)}{\tau} (v^n - v^{n-1}) \right),
\]

\[
\hat{\xi}^{(\tau)}(t) = \left( \hat{F}^{(\tau)}, \hat{Z}^{(\tau)}, \hat{v}^{(\tau)} \right)(t)
\]

\[
= \sum_{n=1}^{\infty} X^n(t) \left( \xi^{n-1} + \frac{t - \tau(n-1)}{\tau} (\xi^n - \xi^{n-1}) \right),
\]

where \( X^n(t) = 1_{[(n-1)\tau, n\tau)} \),

constructed in the time-discrete scheme (2.8) to the solution of elastodynamics before shock formation and provided the error estimate. The proof is based on the relative entropy method [8, 12] and provides an error estimate for the approximation before the formation of shocks. This work is the first step towards numerical method used for practical purposes (eg. computing solutions).

To establish convergence we employed the relative entropy argument (see [8, 12]). We considered the relative entropy,

\[
\eta^r = \frac{1}{2} |\hat{v}^{(\tau)} - v|^2 + \left[ G(\hat{\xi}^{(\tau)}) - G(\xi) - D \xi G(\xi) (\hat{\xi}^{(\tau)} - \xi) \right],
\]

which estimates the difference between time-continuous interpolates \((\hat{v}^{(\tau)}, \hat{\xi}^{(\tau)})\) produced by the scheme and a classical solution \((v, \xi)\) of the enlarged system, and derived the energy identity monitoring the time evolution of \(\eta^r\). I showed that (under appropriate assumptions for growth of \(G\)) the relative entropy \(\eta^r\) satisfies the identity

\[
\partial_t \eta^r - \text{div} \, q^r = Q - \frac{1}{4} D + S \quad \text{in} \quad D',
\]

which monitors its time evolution. Here \(D > 0\) is the dissipation generated by the scheme, \(Q\) is the term equivalent to \(\eta^r\), and \(E\) is the time discretization error. The analysis of the identity yielded the main result: if \((v, F)\) are smooth solutions of the elasticity equations [14] then

\[
\sup_{t \in [0,T]} \left( ||\hat{v}^{(\tau)} - v||^2_{L^2(T^3)} + ||\hat{\xi}^{(\tau)} - \Phi(F)||^2_{L^2(T^3)} + ||\hat{F}^{(\tau)} - F||^p_{L^p(T^3)} \right) = O(\tau).
\]

3 Fully-discrete variational approximation scheme

3.1 Stored energy assumptions

We consider polyconvex stored energy \(W : M_{+}^{3 \times 3} \rightarrow \mathbb{R}\)

\[
W(F) = G \circ \Phi(F), \quad \Phi(F) := (F, \text{cof} F, \det F) \quad \text{(3.1)}
\]

with

\[
G = G(\xi) = G(F, Z, w) : M^{3 \times 3} \times M^{3 \times 3} \times \mathbb{R} \cong \mathbb{R}^{19} \rightarrow \mathbb{R} \quad \text{uniformly convex.}
\]

We work with periodic boundary conditions, that is, the spatial domain \(\Omega\) is taken to be the three dimensional torus \(T^3\). The indices \(i, \alpha, \ldots\) generally run over \(1, \ldots, 3\) while \(A, B, \ldots\) run over \(1, \ldots, 19\). We use the notation \(L^p = L^p(T^3)\) and \(W^{1,p} = W^{1,p}(T^3)\). Finally, we impose the following convexity and growth assumptions on \(G\):

\[
\text{(3.1)}
\]
Remark 3.1. The hypothesis (H1) can be replaced with a more general one
and set the corresponding fields by

\[ G(F) = H_1(F) + H_2(Z) + H_3(w) + R(\xi) \]  

(H1') which leads to a delicate error estimation analysis.

3.2 Motivation for the scheme

In this section we consider fully-discrete scheme induced by the equations (2.8). We first prove an elementary lemma that highlights some of the properties of null-Lagrangians \( \Phi(F) \):

Lemma 3.2 (null-Lagrangian properties). Let \( q > 2 \) and \( r \geq \frac{q}{q-2} \). Then, if

\[ u \in W^{1,q}(\mathbb{T}^3; \mathbb{R}^3), \quad z \in W^{1,r}(\mathbb{T}^3) \]

we have

\[ \partial_a \left( \frac{\partial \Phi_A}{\partial F_{io}}(\nabla u) \right) = 0 \]

\[ \partial_a \left( \frac{\partial \Phi_A}{\partial F_{io}}(\nabla u)z \right) = \frac{\partial \Phi_A}{\partial F_{io}}(\nabla u) \partial_a z \]  

in \( \mathcal{D}'(\mathbb{T}^3) \) 

for each \( i = 1, \ldots, 3 \) and \( A = 1, \ldots, 19 \).
Proof. Observe that
\[
\Phi_{\alpha}(\nabla u) \leq 1 + |\nabla u| + |\nabla u|^2 \Rightarrow \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u) \in L^{q/2}(\mathbb{T}^3).
\]
Hence by (2.2) and the density argument we get (3.5). Next, notice that
\[
\frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u)(z, \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u)\partial_\alpha z) \in L^1(\mathbb{T}^3).
\]
Then taking arbitrary \(\varphi \in C^\infty(\mathbb{T}^3)\) we obtain
\[
\int_{\mathbb{T}^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u)(z) \right) \partial_\alpha \varphi \, dx
= \int_{\mathbb{T}^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u) \right) \partial_\alpha (z \varphi) \, dx - \int_{\mathbb{T}^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u) \partial_\alpha z \right) \varphi \, dx = I_1 - I_2.
\]
Since \(z\varphi \in W^{1,r}_0 \cap W^{1,q}_0\), the property (3.5) and the density argument imply \(I_1 = 0\) and hence
\[
\int_{\mathbb{T}^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u)(z) \right) \partial_\alpha \varphi \, dx = -I_2 = \int_{\mathbb{T}^3} \left( \frac{\partial \Phi^A}{\partial F_{\alpha}}(\nabla u) \partial_\alpha z \right) \varphi \, dx.
\]
Using the above lemma and the properties (P3) and (P4), we conclude that the spatial iterates \(v^n, \xi^n\) constructed in (2.8) solve the system
\[
\frac{v_i^n - v_i^{n-1}}{\tau} = \partial_\alpha \left( \frac{\partial G}{\partial \xi_A}(\xi^n) \frac{\partial \Phi^A}{\partial F_{\alpha}}(F^{n-1}) \right)
\]
\[
\frac{\xi_A^n - \xi_A^{n-1}}{\tau} = \frac{\partial \Phi^A}{\partial F_{\alpha}}(F^{n-1}) \partial_{x_\alpha} v_i^n
\]
which in the shorter form can be expressed
\[
\left( \frac{v_i^n - v_i^{n-1}}{\tau}, \varphi \right) = -\left( D\Phi(\xi^n), D\Phi(F^{n-1})\nabla \varphi \right), \quad \varphi \in C^\infty(\mathbb{T}^3; \mathbb{R}^3)
\]
\[
\left( \frac{\xi_A^n - \xi_A^{n-1}}{\tau}, \psi \right) = \left( D\Phi(F^{n-1})\nabla v_i^n, \psi \right), \quad \psi \in C^\infty(\mathbb{T}^3; \mathbb{R}^{19}).
\]

Remark 3.3. The system (3.6) is equivalent to (2.8) for smooth solutions or functions satisfying (P3)-(P4), but in a distributional sense they are not equivalent. Observe that the product of a function and (possibly) a measure on the right-hand side of the second equation (3.6) may not be defined unless we require \(v\) to have a better regularity.

### 3.3 Fully-discrete scheme and stability

Based on the previous discussion let us investigate a possibility for a fully-discrete scheme based on (3.7). As before, let \(\tau > 0\) be fixed time-step and \(h > 0\) correspond to a space-step. Set
spaces
\[ U_h = \left\{ \varphi_h \in C(T^3; \mathbb{R}^3) : \varphi_h|_K \in [P_h(K)]^3, K \in \mathcal{T}_h(T^3) \right\} \]

\[ H^F_h = \left\{ A_h \in L^2(T^3; M^{3 \times 3}) : A_h|_K \in [P_{h-1}(K)]^9, K \in \mathcal{T}_h(T^3) \right\} \]

\[ H^Z_h = \left\{ B_h \in L^2(T^3; M^{3 \times 3}) : B_h|_K \in [P_{2(h-1)}(K)]^9, K \in \mathcal{T}_h(T^3) \right\} \]

\[ H^w_h = \left\{ d_h \in L^2(T^3) : d_h|_K \in P_{3(h-1)}(K), K \in \mathcal{T}_h(T^3) \right\} \].

and let \( P^U, P^F, P^Z \) and \( P^w \) denote the standard orthogonal projectors,

\[ P^U : L^2(T^3; \mathbb{R}^3) \to U_h \]

\[ P^F : L^2(T^3; M^{3 \times 3}) \to H^F_h \]

\[ P^Z : L^2(T^3; M^{3 \times 3}) \to H^Z_h \]

\[ P^w : L^2(T^3) \to H^w_h , \]

and set the operator \( P^H := (P^F, P^Z, P^w) \).

Consider the following fully-discrete scheme: Given the \((n-1)\)-st iterate

\[ (v_h^{n-1}, \xi_h^{n-1}) = (v_h^{n-1}, F_h^{n-1}, Z_h^{n-1}, w_h^{n-1}) \in U_h \times H^F_h \times H^Z_h \times H^w_h \]

find the \(n\)-th iterate

\[ (v^n_h, \xi^n_h) = (v^n_h, F^n_h, Z^n_h, w^n_h) \in U_h \times H^F_h \times H^Z_h \times H^w_h \]

by solving

\[ \left( \frac{v^n_h - v_h^{n-1}}{\tau}, \varphi_h \right) = -\left( DG(\xi^n_h), D\Phi(F^n_h) \nabla \varphi_h \right), \]

\[ \left( \frac{\xi^n_h - \xi_h^{n-1}}{\tau}, \psi_h \right) = \left( D\Phi(F^n_h) \nabla v^n, \psi_h \right) \]

for all \( \varphi_h \in U_h, \psi_h \in H^F_h \times H^Z_h \times H^F_h \).

Assuming that we are able to solve (3.10) we will try to establish a priori estimates similar to those in (2.9). By assumption

\[ \xi^n_h - \xi_h^{n-1} \in H^F_h \times H^Z_h \times H^w_h \]

and hence

\[ \left( \xi^n_h - \xi_h^{n-1}, P^H DG(\xi^n_h) \right) = \left( \xi^n_h - \xi_h^{n-1}, DG(\xi^n_h) \right) \].

Next, recall that \( \Phi(F) = (F, \text{cof } F, \det F) \) and therefore

\[ \frac{\partial F_{ij}}{\partial F_{j\beta}} = \delta_{ij} \delta_{\alpha\beta}, \quad \frac{\partial (\text{cof } F)_{ij}}{\partial F_{j\beta}} = \epsilon_{ij\kappa} \epsilon_{\alpha\beta\gamma} F_{k\gamma}, \quad \frac{\partial \det F}{\partial F_{j\beta}} = (\text{cof } F)_{j\beta} \]

for each \( i, j, \alpha, \beta = 1, \ldots, 3 \). Then, in view of the fact that

\[ F_h^{n-1} \in H^F_h, \text{cof } (F_h^{n-1}) \in H^Z_h \text{ and } \nabla v^n_h \in H^F_h \]

we conclude that
while by (3.11) and (3.13) we have

This tells us that \( 1 \) and hence, by the convexity of \( G \), which suggest that if \( \phi \) and hence, setting \( \phi \) directly.

Remark 3.4. One actually may avoid introducing orthogonal projector operator (directly). Notice that (3.10) implies that

and therefore

Next, set \( \varphi_h = v_h^n, \psi_h = P^H DG(\xi^n_h) \) and apply it to (3.11). It leads to

which, in view of (3.12) – (3.14), implies

The above identity can be rewritten as

and hence, by the convexity of \( G \), we get an a priori estimate

\[
\frac{1}{2} \| v_h^n \|^2_{L^2(T^3)} + \frac{1}{2} \| v_h^n - v_h^{n-1} \|^2_{L^2(T^3)} + (DG(\xi^n_h), \xi^n_h - \xi^{n-1}_h) = \frac{1}{2} \| v_h^{n-1} \|^2_{L^2(T^3)}
\]

(3.15)

Remark 3.4. One actually may avoid introducing orthogonal projector operator (directly). Notice that (3.10) implies that

while by (3.11) and (3.13) we have

This tells us that

and hence, setting \( \varphi_h = v_h^n \) in (3.10) and using the above identity, we get the same estimate as before.

Finally, notice that the first nine identities in (3.10) are

which suggest that if \( F_h^{n-1} \) is a gradient then \( F^n \) is a gradient, a very useful property if one needs to exploit null-Lagrangian structure; see, e.g., [15].
4 Relative entropy identity

4.1 Relative entropy identity in the smooth regime

In this section we derive the relative entropy identity among the two smooth solutions. This will help to grasp the main idea behind the calculations and, in addition, explain the need for hypotheses (H1)-(H5) on the stored energy \( W(F) \); see Section 4.1. Thus, suppose that

\[
(\hat{v}, \hat{\xi}) = (\hat{v}, \hat{F}, \hat{Z}, \hat{w}), \quad (v, \xi) = (v, F, Z, w)
\]

are two smooth solutions to the extended system (2.4) with \( \hat{F}(\cdot, 0), F(\cdot, 0) \) gradients. Define the relative entropy among the two solutions by

\[
\eta^r(\hat{v}, \hat{\xi}; v, \xi) := \eta(\hat{v}, \hat{\xi}) - \eta(v, \xi) - D\eta(v, \xi)(\hat{v} - v, \hat{\xi} - \xi)
\]

with \( \eta \) given by (2.3). The relative flux in this case will turn out to be

\[
q^r(\hat{v}, \hat{\xi}; v, \xi) := \left( G_{,A}(\hat{\xi}) - G_{,A}(\xi) \right) (\hat{v}_i - v_i) \Phi_{,iA}(\hat{F}).
\]

**Remark 4.1.** Note that (4.1), (4.2) are not symmetrical. Usually, in this type of calculations, \((\hat{v}, \hat{\xi})\) denotes a non-smooth solution which is compared to the smooth \((v, \xi)\). The definition (4.1) ensures that one evaluates gradient \( D\eta \) at the smooth solution to avoid computing the time derivative at the shock (since \( D\eta \) appears in the identity for \( \partial_t \eta^r \)). Also note that the definition of the relative flux \( q^r \) is usually not known in advance and is simply a consequence of computations.

**Lemma 4.2.** Let \((\hat{v}, \hat{\xi})\) and \((v, \xi)\) be smooth solutions of (2.4). Then

\[
\partial_t \eta^r + \partial_{\alpha} q^r_{\alpha} = Q
\]

where the term \( Q \) is "quadratic" of the form

\[
Q(\hat{v}, \hat{\xi}; v, \xi) := \partial_{\alpha} v_i \left( G_{,A}(\hat{\xi}) - G_{,A}(\xi) \right) \left( \Phi_{,iA}(\hat{F}) - \Phi_{,iA}(F) \right) + \partial_{\alpha} \left( G_{,A}(\xi) \right) \left( \Phi_{,iA}(\hat{F}) - \Phi_{,iA}(F) \right) (\hat{v}_i - v_i) + \partial_{\alpha} v_i \left( G_{,A}(\hat{\xi}) - G_{,A}(\xi) - G_{,AB}(\xi)(\hat{\xi} - \xi)_B \right) \Phi_{,iA}(F).
\]

**Proof.** Since \((\hat{v}, \hat{\xi})\) is a smooth solution to (2.4) we have

\[
\partial_t \eta(\hat{v}, \hat{\xi}) = \partial_t \left( \frac{1}{2} |\hat{v}|^2 + G(\hat{\xi}) \right) = \hat{v}_i \partial_{\alpha} \hat{v}_i + G_{,A}(\hat{\xi}) \partial_{\alpha} \hat{\xi}_A
\]

\[
= \hat{v}_i \partial_{\alpha} \left( G_{,A}(\hat{\xi}) \Phi_{,iA}(\hat{F}) \right) + G_{,A}(\hat{\xi}) \partial_{\alpha} \left( \Phi_{,iA}(\hat{F}) \hat{v}_i \right)
\]

\[
= \partial_{\alpha} \left( \hat{v}_i G_{,A}(\hat{\xi}) \Phi_{,iA}(\hat{F}) \right) + G_{,A}(\hat{\xi}) \left( \partial_{\alpha} \left( \Phi_{,iA}(\hat{F}) \hat{v}_i \right) - \Phi_{,iA}(\hat{F}) \partial_{\alpha} \hat{v}_i \right).
\]

Since \( \hat{F}(\cdot, 0) \) is a gradient, (2.4), ensures that it stays gradient. Hence, in view of the null-Lagrangian property (3.5), we have

\[
\partial_{\alpha} \left( \Phi_{,iA}(\hat{F}) \hat{v}_i \right) = \Phi_{,iA}(\hat{F}) \partial_{\alpha} \hat{v}_i
\]

and therefore

\[
\partial_t \eta(\hat{v}, \hat{\xi}) = \partial_{\alpha} \left( \hat{v}_i G_{,A}(\hat{\xi}) \Phi_{,iA}(\hat{F}) \right).
\]
Next, using again (2.4), we get
\[\partial_t \left( \eta(v, \xi) t + D\eta(v, \xi)(\tilde{v} - v, \tilde{\xi} - \xi) \right)\]
\[= \partial_t \left( \frac{1}{2}|v|^2 + G(\xi) + v_i(\tilde{v}_i - v_i) + G_A(\xi)(\tilde{\xi} - \xi)_A \right)\]
\[= \partial_t v_i(\tilde{v}_i - v_i) + G_{,AB}(\xi) \partial_t \xi_B(\tilde{\xi} - \xi)_A + v_i \partial_t \tilde{v}_i + G_A(\xi) \partial_t \tilde{\xi}_A\]
\[= \partial_\alpha \left( G_A(\xi) \Phi^A_{,\alpha}(F) \right)(\tilde{v}_i - v_i)\]
\[+ G_{,AB}(\xi) \partial_\alpha \left( \Phi^B_{,\alpha}(F) v_i \right)(\tilde{\xi} - \xi)_A + v_i \partial_\alpha \left( G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right)\]
\[+ G_A(\xi) \partial_\alpha \left( \Phi^A_{,\alpha}(\tilde{F}) v_i \right).\]

We now modify the above identity by transferring the spatial \(\partial_\alpha\) derivatives onto (what usually is a smooth) solution \((v, \xi)\). This approach and the null-Lagrangian property (3.5) lead us to
\[\partial_t \left( \eta(v, \xi) + D\eta(v, \xi)(\tilde{v} - v, \tilde{\xi} - \xi) \right)\]
\[= \partial_\alpha \left( G_A(\xi) \Phi^A_{,\alpha}(F) \right)(\tilde{v}_i - v_i)\]
\[+ G_{,AB}(\xi) \Phi^B_{,\alpha}(F) \partial_\alpha v_i(\tilde{\xi} - \xi)_A \]
\[+ \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right) - \partial_\alpha v_i \left( G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right)\]
\[+ \partial_\alpha \left( \tilde{v}_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right) - \partial_\alpha \left( G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \tilde{v}_i.\right)\]

Since \(G_{,AB} = G_{BA}\) the second term on the right hand side of (4.6) satisfies
\[G_{,AB}(\xi) \Phi^B_{,\alpha}(F) \partial_\alpha v_i(\tilde{\xi} - \xi)_A = \partial_\alpha v_i \left( G_{,AB}(\xi)(\tilde{\xi} - \xi)_B \right) \Phi^A_{,\alpha}(F)\]
and thus rearranging the terms of (4.6) we obtain
\[\partial_t \left( \eta(v, \xi) + D\eta(v, \xi)(\tilde{v} - v, \tilde{\xi} - \xi) \right)\]
\[= \partial_\alpha \left( G_A(\xi) \left( \Phi^A_{,\alpha}(\tilde{F}) - \Phi^A_{,\alpha}(\tilde{F}) \right) \right)(\tilde{v}_i - v_i)\]
\[- \partial_\alpha v_i \left( G_A(\xi) - G_A(\xi) - G_{,AB}(\xi)(\tilde{\xi} - \xi)_B \right) \Phi^A_{,\alpha}(F)\]
\[+ \partial_\alpha v_i \left( G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right) - \partial_\alpha v_i \left( G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right)\]
\[+ \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right) + \partial_\alpha \left( \tilde{v}_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right).\]

Recalling the definition of the term \(Q\) we see that (4.7) may be written as
\[\partial_t \left( \eta(v, \xi) - D\eta(v, \xi)(\tilde{v} - v, \tilde{\xi} - \xi) \right) =\]
\[= - Q - \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right)\]
\[+ \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right)\]
\[+ \partial_\alpha \left( \tilde{v}_i G_A(\xi) \Phi^A_{,\alpha}(\tilde{F}) \right).\]
Now, we combine (4.5) with (4.8) to get
\[
\partial_t \left( \eta(\hat{v}, \hat{\xi}) - \eta(v, \xi) + D \eta(v, \xi)(\hat{v} - v, \hat{\xi} - \xi) \right) \\
- \partial_\alpha \left( \hat{\nu}_i G_A(\hat{\xi}) \Phi^A_{i,\alpha}(\hat{F}) \right) - \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{i,\alpha}(\hat{F}) \right) \\
+ \partial_\alpha \left( \hat{v}_i G_A(\hat{\xi}) \Phi^A_{i,\alpha}(\hat{F}) \right) + \partial_\alpha \left( \hat{v}_i G_A(\xi) \Phi^A_{i,\alpha}(\hat{F}) \right) = \dot{Q}.
\] (4.9)

Recalling (4.2) we obtain
\[
- \left( \hat{\nu}_i G_A(\hat{\xi}) \Phi^A_{i,\alpha}(\hat{F}) \right) - \partial_\alpha \left( v_i G_A(\xi) \Phi^A_{i,\alpha}(\hat{F}) \right) \\
+ \left( v_i G_A(\xi) \Phi^A_{i,\alpha}(\hat{F}) \right) + \partial_\alpha \left( \hat{v}_i G_A(\xi) \Phi^A_{i,\alpha}(\hat{F}) \right) = \dot{Q}.
\] (4.10)

Then, (4.9) and (4.10) imply the desired identity (4.3).

The identity (4.11) can be used to estimate the evolution of the difference between the two solutions. In particular, one can show that the solution (\hat{v}, \hat{\xi}) stays close to (v, \xi) as long as the initial data do. For this to be realized one would need the "quadratic" term \(Q\) to have the following property:

(GC) If \(M > 0\) is the constant such that
\[
\sup_{(x, t) \in \mathbb{T}^3 \times [0, T]} \left( \sum_{\alpha, i} |\partial_\alpha v_i| + \sum_{\alpha, A} |\partial_\alpha (G_A(\xi))| \right) \leq M,
\] (4.11)

then there holds
\[
|Q(\hat{v}, \hat{\xi}; v, \xi)| \leq C \eta^r(\hat{v}, \hat{\xi}; v, \xi)
\] (4.12)

for some constant \(C = C(M) > 0\) independent of (\(\hat{v}, \hat{\xi}\)).

Indeed, if (GC) is satisfied then one can conclude via the Gronwall lemma that for each smooth solution (\(\hat{v}, \hat{\xi}\)) to (2.4) and fixed smooth solution (\(v, \xi\)) satisfying (4.11) there holds
\[
\int_{\mathbb{T}^3} \left[ \eta^r(\hat{v}, \hat{\xi}; v, \xi) \right] (x, t) \, dx \leq e^{C(M)t} \int_{\mathbb{T}^3} \left[ \eta^r(\hat{v}, \hat{\xi}; v, \xi) \right] (x, 0) \, dx
\] (4.13)

which yields the desired estimate (and guarantees uniqueness of the solution).

Observe that, the inequality (4.12) does not hold in general and also \(Q\) is not necessarily quadratic. One must impose certain requirements on the stored energy \(W = G \circ \Phi\) or more precisely on the function \(G(\xi)\) to satisfy (4.12). On the first glance it seems that it is sufficient to require hypotheses (H2)-(H4) which handle various growth condition and integrability on \(\mathbb{T}^3\). However, splitting the term \(Q\) into two parts as
\[
\begin{align*}
Q(\hat{v}, \hat{\xi}); v, \xi) &= \left[ \partial_\alpha v_i \left( G_A(\hat{\xi}) - G_A(\xi) \right) \left( \Phi^A_{i,\alpha}(\hat{F}) - \Phi^A_{i,\alpha}(F) \right) \right] \\
&+ \left[ \partial_\alpha \left( G_A(\xi) \right) \left( \Phi^A_{i,\alpha}(\hat{F}) - \Phi^A_{i,\alpha}(F) \right) \right] \hat{v}_i - v_i \\
&+ \partial_\alpha v_i \left( G_A(\hat{\xi}) - G_A(\xi) - G_A(\xi)(\hat{\xi} - \xi) \right) B \Phi^A_{i,\alpha}(F) \right] =: Q_1 + Q_2,
\end{align*}
\] (4.14)

we find that \(Q_1\) (the last 10 terms in its sum) fails to comply with (GC) regardless of (H2)-(H4).

To satisfy (GC) there are two options to consider:
(O1) One can assume (H1) which implies (GC). The hypothesis (H1) is used in [15] to handle the convergence in the semi-discrete case. The advantage of (H1) is that it allows to work with a very concrete class of functions. The disadvantage is that it restricts the class of stored energies even though allows for $L^p$ growth in $\tilde{F}$ component. The reviewer of [15] noticed to me that perhaps it is best to work with more general class of stored energies. Namely, it holds exactly, that is, (4.15) is equivalent to

$$\int_{\Omega_3} \frac{v_{i,h}^n - v_{i,h}^{n-1}}{\tau} \varphi_i^h dx = - \int_{\Omega_3} \left( G_{,A}(\xi^n_{A,h}) \Phi_{,\alpha}^A(F^n_{h-1}) \right) \partial_\alpha \varphi_i^h dx$$

for all $\alpha \in U_h$, $\psi_h = (\psi_{A,h})_{A=1}^{10} \in H_h := H_h^F \times H_h^Z \times H_h^w.$

The choice of finite element spaces has a great impact on the fully discrete scheme. Namely, the space $H_h$ of test functions turned out to be so rich (c.f. (3.16)) that the last equation in (4.15) holds exactly, that is, (4.15) is equivalent to

$$\int_{\Omega_3} \frac{v_{i,h}^n - v_{i,h}^{n-1}}{\tau} \varphi_i^h dx = - \int_{\Omega_3} \left( G_{,A}(\xi^n_{A,h}) \Phi_{,\alpha}^A(F^n_{h-1}) \right) \partial_\alpha \varphi_i^h dx$$

for all $\varphi_i^h = (\varphi_i^h)_{i=1}^{3} \in U_h$.

**Remark 4.3.** The scheme in the form (4.16) provides a great opportunity to us since we are able to exploit the null-Lagrangian properties. Namely, (4.16) guarantees that if $F^n_h$ is a gradient then $F^n_h$, $n \geq 1$ are all gradients as well and hence the null-Lagrangian properties could be exploited regardless of $F^n$ being discontinuous; see Lemma 3.2. For example, when $y(x,t)$ is a smooth map that induces initial data

$$v_0(x) = \partial_t y(x,0), \quad F_0 = \nabla y(x,0).$$

we set

$$F^n_h := \nabla(P^n y(x,0)) \in H^F$$

where $P^n$ is a standard $L^2$-projector on $U_h$ defined in (3.3).
Approximates. Given the sequence of spatial iterates \((v^n_h, \xi^n_h)\), \(n \geq 1\) we define (following [15]) the time-continuous, piecewise linear interpolates
\[
\hat{\Theta}^{(\tau,h)} := (\hat{v}^{(\tau,h)}, \hat{\xi}^{(\tau,h)})
\]
with
\[
\hat{v}^{(\tau,h)}(t) = \sum_{n=1}^{\infty} \mathcal{X}^n(t) \left( v^{n-1}_h + \frac{t - \tau(n - 1)}{\tau}(v^n_h - v^{n-1}_h) \right)
\]
\[
\hat{\xi}^{(\tau,h)}(t) = \left( \hat{F}^{(\tau,h)}, \hat{Z}^{(\tau,h)}, \hat{u}^{(\tau,h)} \right)(t)
\]
\[
= \sum_{n=1}^{\infty} \mathcal{X}^n(t) \left( \xi^{n-1}_h + \frac{t - \tau(n - 1)}{\tau}(\xi^n_h - \xi^{n-1}_h) \right),
\]
and the piecewise constant interpolates
\[
\tilde{\Theta}^{(h)} := (\tilde{v}^{(\tau,h)}, \tilde{\xi}^{(\tau,h)}) \quad \text{and} \quad \tilde{F}^{(\tau,h)}
\]
by
\[
\tilde{v}^{(\tau,h)}(t) = \sum_{n=1}^{\infty} \mathcal{X}^n(t)v^n_h
\]
\[
\tilde{\xi}^{(\tau,h)}(t) = \left( \tilde{F}^{(\tau,h)}, \tilde{Z}^{(\tau,h)}, \tilde{u}^{(\tau,h)} \right)(t) = \sum_{n=1}^{\infty} \mathcal{X}^n(t)\xi^n_h
\]
\[
\tilde{F}^{(\tau,h)}(t) = \sum_{n=1}^{\infty} \mathcal{X}^n(t)F^n_{\tau,n\tau}^{-1},
\]
where \(\mathcal{X}^n(t)\) is the characteristic function of the interval \(I_n := [(n-1)\tau, n\tau)\). Notice that \(\tilde{F}^{(\tau,h)}\) is the time-shifted version of \(F^{(\tau,h)}\) and used later in various calculations.

The scheme via approximates. Clearly the linear approximates (4.19) are absolutely continuous in time. This motivates to rewrite the discrete system (4.16) in terms of the approximates (4.19), (4.20). Then the scheme (4.16) transforms into:
\[
\int_{\mathbb{T}^3} \left( \partial_i \tilde{v}^{(\tau,h)}_i \right) \varphi_h^i \, dx = - \int_{\mathbb{T}^3} \left( G_{i\alpha}(\tilde{\xi}^{(\tau,h)}) \Phi_{i\alpha}^{\tilde{F}^{(\tau,h)}} \right) \partial_{\alpha} \varphi_h^i \, dx
\]
\[
\partial_t \tilde{\xi}^{(\tau,h)} = \Phi_{i\alpha}^{\tilde{F}^{(\tau,h)}} \partial_{\alpha} \tilde{v}^{(\tau,h)}_i
\]
for a.e. \(t > 0\) and \(\forall \varphi_h = (\varphi_h^i)_{i=1}^3 \in U_h\).

4.3 Stability of the fully-discrete variational scheme

For the rest of the sequel, we suppress the dependence on \(\tau, h\) to simplify notations and assume that:

(A1) \(\hat{\Theta} = (\hat{v}, \hat{\xi})\) are the time-continuous approximates; see (4.19).

(A2) \(\hat{\Theta} = (\hat{v}, \hat{\xi})\) and \(\hat{F}\) are the constant approximates; see (4.20).

(A3) \(\Theta = (v, \xi) = (v, F, Z, w)\) is a smooth solution to (2.4) on \(\mathbb{T}^3 \times [0, T]\).

(A4) \(F^0, F(\cdot, 0)\) are gradients and initial iterate \((v^0, \xi^0) \in U_h \times H_h\).

The goal of this section is to derive an identity for a relative energy among the two solutions. To this end, we define the relative entropy
\[
\eta^\tau(\hat{\Theta}, \Theta) := \eta(\hat{\Theta}) - \eta(\Theta) - D\eta(\Theta)(\hat{\Theta} - \Theta)
\]
(4.22)
where $\eta$ is the convex entropy of the extended elasticity system \([2, 4]\) defined by

$$
\eta(\Theta) = \frac{1}{2}|v|^2 + G(\xi), \quad \Theta = (v, \xi).
$$

(4.23)

To deriving the relative entropy identity, we will employ the lemma \([3, 2]\) that extends the null-Lagrangian properties to non-smooth gradients. These properties will be used extensively in our computations throughout the paper.

**Lemma 4.4 (relative entropy identity).** Let (A1)-(A4) hold. Then

$$
\int_{\mathbb{T}^3} \partial_t \eta^r(x, t) \, dx = \int_{\mathbb{T}^3} \left( -\frac{1}{\tau} D + Q + E + \bar{E} \right) \, dx, \quad \text{a.e. } t \in [0, T]
$$

(4.24)

where

$$
Q := \partial_\alpha (G, A(\xi))(\Phi_{i\alpha}^A(\hat{F}) - \Phi_{i\alpha}^A(F))(\hat{v}_i - v_i)
$$

$$
+ \partial_\alpha v_i (G, A(\hat{\xi}) - G, A(\xi))(\Phi_{i\alpha}^A(\hat{F}) - \Phi_{i\alpha}^A(F))
$$

$$
+ \partial_\alpha v_i (G, A(\hat{\xi}) - G, A(\xi) - G, AB(\xi)(\hat{\xi} - \xi) \nu)(\Phi_{i\alpha}^A(F))
$$

(4.25)

estimates the difference between the two solutions,

$$
D := \sum_{n=1}^{\infty} \chi_n(t) D^n \quad \text{with} \quad D^n := (\nabla \eta(\hat{\Theta}) - \nabla \eta(\hat{\Theta})) \delta \Theta^n,
$$

(4.26)

where

$$
\delta \Theta^n = (\delta v^n, \delta F^n, \delta Z^n, \delta w^n) := \Theta^n - \Theta^{n-1}
$$

$$
= (v^n - v^{n-1}, F^n - F^{n-1}, Z^n - Z^{n-1}, w^n - w^{n-1}),
$$

(4.27)

is the dissipative term,

$$
E := \partial_\alpha (G, A(\xi)) \left[ \Phi_{i\alpha}^A(F)(\hat{v}_i - v_i)
$$

$$
+ (\Phi_{i\alpha}^A(\hat{F}) - \Phi_{i\alpha}^A(F))(\hat{v}_i - v_i)
$$

$$
+ (\Phi_{i\alpha}^A(\hat{F}_s) - \Phi_{i\alpha}^A(F))(\hat{v}_i - v_i)
$$

$$
+ (\Phi_{i\alpha}^A(\hat{F}) - \Phi_{i\alpha}^A(F))(\hat{v}_i - v_i) \right]
$$

(4.28)

is the error term that appears due to the discretization in time, and

$$
\bar{E} := G, A(\hat{\xi}) \Phi_{i\alpha}^A(\hat{F}_s) \partial_\alpha ((\nabla^2 v)_i - v_i)
$$

(4.29)

is the error term that appears due to spatial discretization.

**Proof.** By (A1) we have that $F^0_h, F(\cdot, 0)$ are gradients. Hence by \([4.10, 4.19, 4.20]\), and the property (E1) we conclude

$$
\hat{F}, \hat{F}, \hat{F}_s \text{ and } F \text{ are gradients } \forall t \in [0, T].
$$

(4.30)
Next, recalling (4.34) we compute
\[
\partial_t (\eta(\Theta)) = \tilde{v}_i \partial_i \tilde{v}_i + G_{,A}(\xi) \partial_i \tilde{\xi}_A
\]
\[
= \tilde{v}_i \partial_i \tilde{v}_i + G_{,A}(\xi) \partial_i \tilde{\xi} + \frac{1}{r} \sum_{n=1}^{\infty} X^n(t)(\nabla \eta(\Theta) - \nabla \eta(\Theta)) \delta \Theta^n.
\]  
(4.31)

By construction \( \tilde{v}(\cdot, t) \in U_h, \forall t \in [0, t] \). Thus, setting \( \varphi = \tilde{v}(\cdot, t) \) in the weak formulation (4.21) and using (4.21) we obtain
\[
\int_{T^3} \tilde{v}_i \partial_i \tilde{v}_i \, dx = - \int_{T^3} G_{,A}(\xi) \Phi_{,\alpha}^A(F) \partial_\alpha \tilde{v}_i \, dx = - \int_{T^3} G_{,A}(\xi) \partial_t \tilde{\xi} \, dx.
\]

Then, integrating expression (4.31) we obtain
\[
\int_{T^3} \partial_t (\eta(\Theta)) \, dx = \int_{T^3} \left(- \frac{1}{r} \sum_{n=1}^{\infty} X^n(t)(\nabla \eta(\Theta) - \nabla \eta(\Theta)) \delta \Theta^n\right) \, dx.
\]  
(4.32)

Next, we compute
\[
\partial_t \left( \frac{1}{2} v^2 + G(\xi) + v_i (\tilde{v}_i - v_i) + G_{,A}(\xi) (\tilde{\xi} - \xi) A \right) = \partial_t v_i (\tilde{v}_i - v_i) + \partial_i (G_{,A}(\xi)) (\tilde{\xi} - \xi) A + v_i \partial_i v_i + G_{,A}(\xi) \partial_i \tilde{\xi}_A.
\]
(4.33)

Since \((v, \xi)\) is a smooth solution to (2.4) we have
\[
\partial_t v_i = \partial_i (G_{,A}(\xi) \Phi_{,\alpha}^A(F)) = \partial_i (G_{,A}(\xi)) \Phi_{,\alpha}^A(F)
\]
\[
\partial_t \tilde{\xi}_A = \partial_\alpha (\Phi_{,\alpha}^A(F) v_i) = \Phi_{,\alpha}^A(F) \partial_\alpha v_i
\]
where we used (3.5) and the fact that \(F\) is a gradient. Also, from (4.16) and (4.21) it follows that \(\partial_t \tilde{v} \in U_h\). Hence, since \(P^l\) is a standard orthogonal projector, by (4.21) we have
\[
\int_{T^3} v_i \partial_i \tilde{v}_i \, dx = \int_{T^3} (P^l v_i) \partial_i \tilde{v}_i \, dx = - \int_{T^3} G_{,A}(\tilde{\xi}) \Phi_{,\alpha}^A(F) \partial_\alpha (P^l v_i) \, dx.
\]

Finally, by (4.21)
\[
\int_{T^3} G_{,A}(\xi) \partial_i \tilde{\xi}_A \, dx = \int_{T^3} G_{,A}(\xi) \Phi_{,\alpha}^A(F) \partial_\alpha \tilde{v}_i \, dx.
\]

Now, integrating (4.33) and using the last four identities we get
\[
\int_{T^3} \partial_t (\eta(\Theta) + \nabla \eta(\Theta)(\tilde{\Theta} - \Theta)) \, dx = \\
\int_{T^3} \partial_\alpha (G_{,A}(\xi)) \Phi_{,\alpha}^A(F) (\tilde{v}_i - v_i) \, dx \\
+ \int_{T^3} G_{,AB}(\xi) \Phi_{,\alpha}^B(F) \partial_\alpha v_i (\tilde{\xi} - \xi) A \, dx \\
+ \int_{T^3} \left(G_{,A}(\xi) \Phi_{,\alpha}^A(F) \partial_\alpha \tilde{v}_i - G_{,A}(\xi) \Phi_{,\alpha}^A(F) \partial_\alpha v_i\right) \, dx \\
+ \int_{T^3} G_{,A}(\tilde{\xi}) \Phi_{,\alpha}^A(F) \partial_\alpha (v_i - (P^l v_i)) \, dx.
\]  
(4.34)

Subtracting (4.34) from (4.31), recalling (4.22), (4.20) and (4.29), and then using the fact that \(G_{,AB} = G_{BA}\) we conclude that
\[
\int_{T^3} \eta'(x, t) \, dx = \int_{T^3} \left(- \frac{1}{r} \sum_{n=1}^{\infty} X^n(t) D_n + \tilde{E} + J\right) \, dx
\]  
(4.35)
with
\[ J := \partial_\alpha v_i \left( G_{A,\xi} - G_{A,\xi}(\xi) - G_{A,\xi}(\xi) (\xi - \xi_B) \right) \Phi_{i,\alpha}^A(F) \]
\[ + \partial_\alpha v_i \left[ \left( G_{A,\xi} - G_{A,\xi}(\xi) \right) \Phi_{i,\alpha}^A(F) - \left( G_{A,\xi}(\xi) - G_{A,\xi}(\xi) \right) \Phi_{i,\alpha}^A(F) \right] \]
\[ + \partial_\alpha (G_{A,\xi}(\xi)) \left( \Phi_{i,\alpha}^A(F_\ast)(\xi - \xi_B) \right) \]
\[ + \Phi_{i,\alpha}^A(F)(\xi - \xi_B) \]
\[ := J_1 + J_2 + J_3 + J_4. \]

Consider the terms on the right-hand side of (4.36). First, we rearrange the term \( J_2 \) as follows
\[ J_2 = \partial_\alpha v_i \left[ \left( G_{A,\xi} - G_{A,\xi}(\xi) \right) \Phi_{i,\alpha}^A(F_\ast) \right] \]
\[ = \partial_\alpha v_i \left[ \left( G_{A,\xi} - G_{A,\xi}(\xi) \right) \Phi_{i,\alpha}^A(F_\ast) \right] \]
\[ + \partial_\alpha (G_{A,\xi}(\xi)) \left( \Phi_{i,\alpha}^A(F_\ast) - \Phi_{i,\alpha}^A(F) \right) \]
\[ + \Phi_{i,\alpha}^A(F)(\xi - \xi_B) \]
\[ (4.37) \]
\[ J_3 = \partial_\alpha (G_{A,\xi}(\xi)) \left[ \Phi_{i,\alpha}^A(F_\ast)(\xi - \xi_B) \right] \]
\[ = \partial_\alpha (G_{A,\xi}(\xi)) \left[ \Phi_{i,\alpha}^A(F_\ast)(\xi - \xi_B) \right] \]
\[ + \Phi_{i,\alpha}^A(F)(\xi - \xi_B) \]
\[ (4.38) \]
\[ J_4 = \partial_\alpha v_i \left[ \left( G_{A,\xi} - G_{A,\xi}(\xi) \right) \Phi_{i,\alpha}^A(F) \right] \]
\[ \ast \]
\[ + \Phi_{i,\alpha}^A(F)(\xi - \xi_B) \]
\[ := J_1 + J_2 + J_3 + J_4. \]

Then, we modify the term \( J_3 \) writing it in the following way:
\[ J_3 = \partial_\alpha (G_{A,\xi}(\xi)) \left[ \Phi_{i,\alpha}^A(F_\ast)(\xi - \xi_B) \right] \]
\[ = \partial_\alpha (G_{A,\xi}(\xi)) \left[ \Phi_{i,\alpha}^A(F_\ast)(\xi - \xi_B) \right] \]
\[ + \Phi_{i,\alpha}^A(F)(\xi - \xi_B) \]
\[ (4.39) \]
\[ \text{in the sense that} \]
\[ - \int_{T^3} \sum_{\alpha=1}^3 \left( \frac{\partial \Phi_{i,\alpha}^A}{\partial F_{i,\alpha}}(F_\ast)(v_i - \tilde{v}_i) \right) \partial_\alpha \phi \, dx = \]
\[ \int_{T^3} \sum_{\alpha=1}^3 \left( \frac{\partial \Phi_{i,\alpha}^A}{\partial F_{i,\alpha}}(\tilde{F}_\ast)(v_i - \tilde{v}_i) \right) \partial_\alpha \phi \, dx, \quad \forall \phi \in C^\infty(T^3). \]
\[ (4.40) \]

By the standard density argument (4.40) holds for all \( \phi \in W^{1,1}(T^3) \). Since \( \xi \) is smooth, we have \( \phi_A := G_{A,\xi}(\xi, t) \in C^1(T^3) \). Then, considering (4.40) with \( \phi_A \) for each \( A = 1, \ldots, 19 \) and
summing over \( i = 1, \ldots, 3 \) and \( A = 1, \ldots, 19 \) (using the summation convention over repeated indices) we conclude

\[
0 = \int_{T^3} \Phi_{,iA}(\tilde{F}_s)(v_i - \tilde{v}_i) \partial_\alpha (G_{,A}(\xi)) \, dx \\
+ \int_{T^3} \Phi_{,iA}(\tilde{F}_s) \partial_\alpha (v_i - \tilde{v}_i) G_{,A}(\xi) \, dx = \int_{T^3} J_4 \, dx.
\] (4.41)

Finally, combining (4.36)-(4.38) and (4.41) we conclude

\[
\int_{T^3} J \, dx = \int_{T^3} (J_1 + J_2 + J_3 + J_4) \, dx = \int_{T^3} (Q + E) \, dx
\] (4.42)

with terms \( Q, E \) defined in (4.25), (4.28) respectively. Then (4.35), (4.42) imply the desired identity (4.24).

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