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DOI
10.1016/j.cma.2019.112664

Publication date
2020

Document Version
Accepted author manuscript

Published in
Computer Methods in Applied Mechanics and Engineering

A theoretical framework for discontinuity capturing: Joining variational multiscale analysis and variation entropy theory

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Abstract

In this paper we show that the variational multiscale method together with the variation entropy concept form the underlying theoretical framework of discontinuity capturing. The variation entropy [M.F.P ten Eikelder and I. Akkerman, Variation entropy: a continuous local generalization of the TVD property using entropy principles, Comput. Methods. Appl. Mech. Engrg. 355 (2019) 261-283, 2019] is the recently introduced concept that equips total variation diminishing solutions with an entropy foundation. This is the missing ingredient in order to show that the variational multiscale method can capture sharp layers. The novel framework *naturally* equips the variational multiscale method with a class of discontinuity capturing operators. This class includes the popular YZβ method and methods based on the residual of the variation-entropy. The discontinuity capturing mechanisms do not contain *ad hoc* devices and appropriate length scales are derived. Numerical results obtained with quadratic NURBS are virtually oscillation-free and show sharp layers, which confirms the viability of the methodology.

Keywords: Discontinuity capturing operators, Variational multiscale method, Variation entropy, TVD property, Variation entropy residual-based, Isogeometric analysis

1. Introduction

Discontinuities in physical quantities such as densities, pressures and velocities often occur in scientific and industrial problems. Common examples include explosions, cavitation events, two-fluid flows and traffic congestion. These phenomena are generally modeled by (nonlinear) conservation laws. Numerical methods that aim to solve these conservation laws encounter difficulties at the shock waves. Straightforward discretizations pollute the discrete solution by spurious oscillations. To overcome this, the numerical method typically introduces additional diffusion/viscosity near the shock. There exist many possibilities, depending on the underlying numerical method, on how to determine this diffusion term.

In the finite-difference and finite-volume world, additional diffusion is often the result of one of the following approaches. Perhaps the simplest technique to introduce diffusion is to use a standard upwind method. This removes the spurious oscillations, but the price one has to pay is a significant decrease of accuracy. An alternative is to use a monotonic upwind scheme for conservation laws (MUSCL) [1–4], also known as a limiter scheme, which reduces the numerical flux to first-order near the shock. Several other approaches equip the numerical method with discrete features. Examples include schemes with the monotonicity property [5], the total variation diminishing schemes [5–7] or methods that ensure the maximum principle [5, 8], e.g. in two-fluid flow simulations [9–11].

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In the context of finite element methods, the spurious wiggles were first addressed with the Streamline upwind-Petrov Galerkin (SUPG) method for incompressible flow problems in the well-known 1982 paper [12] and for compressible flow problems in [13, 14]. The compressible flow case required a quasi-linear form which leads to the concept of generalized advection operators. In both cases the SUPG method adds diffusion only in the direction of the flow and is not subject to artificial diffusion criticism. The SUPG method provides accurate solutions without oscillations when strong shocks are absent. In regions near sharp layers a more robust formulation was needed. To this purpose, several shock capturing operator mechanisms are introduced. One of the first of these techniques has been proposed in [15]. This method provides control of gradient of the solution. The sharp layers in compressible flows were addressed by Hughes et al. who proposed to use entropy variables [16] and entropy variables in combination with the SUPG operator [17, 18]. Le Beau and Tezduyar equipped the original SUPG method with a shock capturing operator in conservative variables [19, 20]. The numerical computations reveal that results of using entropy variables without shock-capturing are nearly indistinguishable from using conservative variables with shock-capturing [20]. This might indicate a similarity or relation between shock capturing methods and entropy variables. Another important discontinuity capturing method is $YZ\beta$ shock-capturing [21–24]. This shock-capturing is based on scaled residuals and contains user-defined parameters which can be chosen depending on the smoothness of the layer. Other work on discontinuity capturing includes the CAU method [25] in which the flow velocity in the SUPG term is replaced by an approximate upwind direction and the work of Sampaio and Coutinho [26] in which an effective transport velocity is used. For a more complete overview of stabilized methods and shock capturing techniques for compressible flows we refer to the review papers [27–29].

A particular class of stabilized finite element methods is that of the variational multiscale methods [30–32]. The idea is to incorporate the effect of the small-scales via a model equation in the resolved part of the solution. This improves the stability of the finite element scheme. This framework provides a theoretical foundation of stabilized methods. It has been widely applied for the computation of incompressible turbulence [33–40]. The corresponding turbulence model is residual-based and does not contain ad-hoc mechanisms. The technique finds also applications in free-surface flow and FSI computations [41–44]. The multiscale formulation is often augmented with an artificial discontinuity capturing term when sharp layer may occur. The VMS method offers rich possibilities to design new methods. It can be used to enforce a particular property in the numerical method, such as a total variation bounding constraint [45] and the maximum principle [46]. Other recent work includes a VMS method that employs particular fine-scale models to arrive at a discontinuity capturing term [47].

More recently a popular discontinuity capturing method known by the name *entropy viscosity method* has been introduced [48]. This method bases the added nonlinear viscosity on the entropy residual. The motivation originates from the fact the entropy satisfies a conservation equation in smooth regions and an inequality in at shock waves. Basing the viscosity on the entropy production does not affect the smooth regions while in shock regions numerical dissipation is added. The entropy viscosity method has been further developed in the framework of discontinuous Galerkin methods in [49]. Furthermore, the stability of explicit entropy viscosity methods has been analyzed [50]. The method is a promising technique and has shown quite well behavior on many benchmark problems. It is however an heuristic approach for which, to the best knowledge of the authors, the theoretical justification is still missing. We cite

Guermond et al. [48]: '*the amount of theory to justify the approach is almost non-existent. The justification of the method is mainly heuristic for the time being.*'.

The idea of using an entropy concept to locate sharp layers is interesting. We have recently proposed the variation entropy theory [51] which provides entropy solutions with a new perspective and can be viewed an extension of total variation diminishing solutions. In order to identify sharp layers in solution profiles, the idea is to look at the gradient of the solution instead of at the solution itself. The variation entropy concept provides an entropy framework to analyze the behavior of the gradient of the solution using the so-called variation entropy condition. In a numerical setting this can be a tool to locate Gibbs oscillations.

All the previously mentioned techniques that add numerical diffusion in the region of the sharp layer are in some way the result of equipping the method with a favorable numerical property. The methods are *ad hoc* technologies that are not derived from the continuous partial differential equation. We note that Bazilevs et al. [24] conjecture that the variational multiscale method is the correct theoretical groundwork for discontinuity capturing methods:

Bazilevs et al. [24]: '*While stabilized methods may be derived on the basis of the variational multiscale methodology, discontinuity capturing is an ad hoc technique. Nevertheless, it is a widely used technology that enables a practitioner to successfully tackle real-world applications. We believe that the multiscale framework with a proper set of optimality conditions is the right underlying theoretical structure that may more naturally lead to discontinuity capturing formulations. This conjecture is intriguing and warrants further investigation.*'.

In the current paper we prove that this conjecture is valid. To establish this, we unify previous ideas and concepts into a variational multiscale-variation entropy framework. We believe that the variation entropy theory was the missing element in order to be able to demonstrate the correctness of the conjecture in [24]. The variation entropy idea tells us the location of the viscosity whereas the multiscale concept provides a way to model the viscosity via the missing scales. Merging the variational multiscale method with the variation entropy framework *naturally* augments the VMS method with a discontinuity capturing operator. We sketch this in Figure 1. We propose a discontinuity capturing viscosity that is variation-entropy residual-based. In some sense this is similar to the entropy viscosity method [48] where the residual is based on the entropy. In contrast, our discontinuity capturing term comes with theoretical foundations. We emphasize that the proposed framework does not contain *ad hoc* devices. The approximate small-scale models are physics-based by means of Green's functions and residuals.

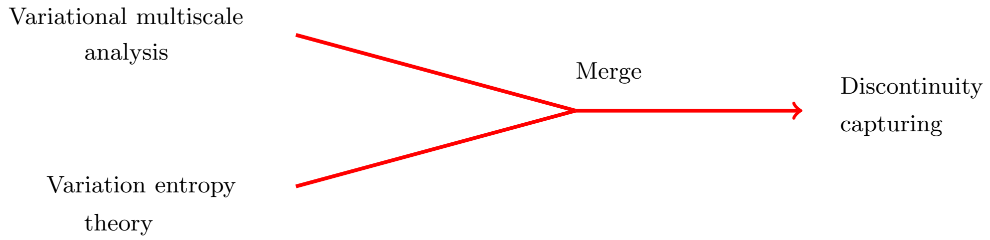


Figure 1: Merging the variational multiscale method and the variation entropy concept leads to a discontinuity capturing term

The remainder of the paper can be summarized as follows. The Section 2 briefly introduces the notion of entropy and variation entropy solutions. In Section 3 we present the discontinuity capturing framework based on the variational multiscale analysis and variation entropy theory. Section 4 presents numerical results and in Section 5 we draw the conclusions and outline avenues for future research.

2. Entropy solutions

2.1. The classical entropy

Let $\Omega \subset \mathbb{R}^d$ be an open and connected domain. Consider the scalar-valued conservation problem:

find $\phi : \Omega \times \mathcal{I} \to \mathbb{R}$ *such that*

$$\partial_t \phi + \nabla \cdot \mathbf{f} = 0, \qquad (\mathbf{x}, t) \in \Omega \times \mathcal{I}, \tag{1a}$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}). \tag{1b}$$

The problem is equipped with appropriate boundary conditions. We assume that the initial condition $\phi_0 \in L^\infty(\Omega)$ has compact support in Ω. The smooth (nonlinear) flux denotes $\mathbf{f} = \mathbf{f}(\phi)$, the spatial coordinate is $\mathbf{x} \in \Omega$ and time is $t \in \mathcal{I} = (0, t_e)$ with $t_e > 0$. The problem (1) can produce discontinuities and shocks which motivates the usage of weak solutions. A weak solution ϕ is a bounded function that satisfies

$$\int_0^\infty \int_\Omega (\phi \partial_t v + \mathbf{f} \cdot \nabla v)\, \mathrm{d}\mathbf{x}\mathrm{d}t + \int_\Omega \phi_0(\mathbf{x}) v(\mathbf{x}, 0) \mathrm{d}\mathbf{x} = 0, \tag{2}$$

for all test functions $v \in \mathcal{C}_c^\infty(\Omega \times [0, \infty])$ (i.e. v is smooth and has compact support). An important observation is that physically and mathematically correct solutions are vanishing viscosity solutions. This is a key ingredient in the concept of *entropy solutions* which are weak solutions that satisfy an additional inequality, denoted as the *entropy condition*.

Definition 2.1. *A solution of (1) is called an entropy solution if it satisfies, in the distributional sense, the entropy condition:*

$$\partial_t \eta(\phi) + \nabla \cdot \mathbf{q}(\phi) \leq 0, \tag{3}$$

for all convex entropy functions η. Condition (3) is rigorously understood as

$$\int_0^\infty \int_\Omega (\eta(\phi) \partial_t v + \mathbf{q}(\phi) \cdot \nabla v)\, \mathrm{d}\mathbf{x}\mathrm{d}t \geq 0, \tag{4}$$

for all test functions $v \in \mathcal{C}_c^\infty(\Omega \times [0, \infty]), v \geq 0$.

Definition 2.2. *A pair of functions $(\eta, \mathbf{q}) = (\eta(\phi), \mathbf{q}(\phi))$ is called an entropy-entropy flux pair for the conservation law (1) if*

- *η is convex*
- *the compatibility condition is satisfied:*

$$\frac{\partial \mathbf{q}}{\partial \phi} = \frac{\partial \eta}{\partial \phi} \frac{\partial \mathbf{f}}{\partial \phi}. \tag{5}$$

For smooth solutions the entropy condition is satisfied with equality, while the entropy dissipates at shock waves. In absence of boundary conditions, integration of (3) over Ω leads to a dissipation of the overall entropy:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \eta(\phi)\ \mathrm{d}\Omega \leq 0 \Rightarrow \int_\Omega \eta(\phi(\mathbf{x}, t))\ \mathrm{d}\Omega \leq \int_\Omega \eta(\phi_0(\mathbf{x}))\ \mathrm{d}\Omega, \quad \text{for all } t > 0. \tag{6}$$

This *a-priori* estimate is the so-called entropy stability property and can be understood as a nonlinear L^2-stability for conservation laws when taking $\eta(\phi) = \phi^2/2$.

Theorem 2.3. *Entropy solutions are unique (in the scalar case).*

Proof. See [52, 53]. □

For more details about entropy solutions one can consult e.g. [52–55].

2.2. The variation entropy

The idea of the variation entropy (VE), developed in [51], is to consider the entropy of the conservation law of $\nabla\phi$ instead of ϕ. We start off with the same conservation law:

find $\phi : \Omega \times \mathcal{I} \to \mathbb{R}$ such that

$$\partial_t \phi + \nabla \cdot \mathbf{f} = 0, \qquad (\mathbf{x}, t) \in \Omega \times \mathcal{I}, \tag{7a}$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}). \tag{7b}$$

in which the initial condition $\phi(\mathbf{x},0) = \phi_0(\mathbf{x}) \in L^\infty(\Omega)$ is assumed to have compact support. The flux $\mathbf{f} = \mathbf{f}(\phi) \in \mathcal{C}(\Omega,\mathbb{R})$ is possibly nonlinear.

Remark 2.4. In this paper we restrict ourselves to the hyperbolic case, i.e. $\mathbf{f} = \mathbf{f}(\phi)$, unless explicitly indicated. It is also possible to consider the parabolic case in which the flux depends on $\nabla\phi$, i.e. $\mathbf{f} = \mathbf{f}(\phi, \nabla\phi)$. In that case one needs to assume that the matrix $\partial\mathbf{f}/\partial\nabla\phi$ is symmetric negative definite.

Definition 2.5. *The convex function $\eta = \eta(\nabla\phi)$ is said to be a variation entropy if $\eta(\mathbf{0}) = 0$ and it satisfies the variation entropy condition*

$$\partial_t\eta + \nabla\cdot\mathbf{q} \leq 0, \tag{8}$$

in weak sense where the flux $\mathbf{q}$ satisfies the compatibility condition

$$\mathbf{q} = \frac{\partial\mathbf{f}}{\partial\phi}\nabla\phi\cdot\frac{\partial\eta}{\partial\nabla\phi}. \tag{9}$$

Remark 2.6. For parabolic problems the variation entropy condition reads

$$\partial_t\eta + \nabla\cdot\mathbf{q} - \mathscr{D} \leq 0, \tag{10}$$

in weak sense where the flux $\mathbf{q}$ and the non-conservative term $\mathscr{D}$ are respectively given by:

$$\mathbf{q} = \frac{\partial\mathbf{f}}{\partial\phi}\nabla\phi\cdot\frac{\partial\eta}{\partial\nabla\phi} + \frac{\partial\mathbf{f}}{\partial\nabla\phi}\nabla\eta, \tag{11a}$$

$$\mathscr{D} = (\mathbf{H}_\mathbf{x}\phi\mathbf{H}_{\nabla\phi}\eta) : \left(\frac{\partial\mathbf{f}}{\partial\nabla\phi}\mathbf{H}_\mathbf{x}\phi\right). \tag{11b}$$

Here $\mathbf{H}_\mathbf{x}\phi$ and $\mathbf{H}_{\nabla\phi}\eta$ are the Hessians of ϕ and η.

Proposition 2.7. *A variation entropy satisfies the homogeneity property:*

$$\mathbf{v}\cdot\frac{\partial\eta}{\partial\mathbf{v}} = \eta, \qquad \textit{for all } \mathbf{v}\in\mathbb{R}^d. \tag{12}$$

Theorem 2.8. *A function η is a variation entropy if and only if*

- *η is positive homogeneous function of degree 1:*

$$\eta(\gamma\mathbf{v}) = \gamma\eta(\mathbf{v}) \qquad \textit{for all } \gamma\geq 0, \mathbf{v}\in\mathbb{R}^d. \tag{13}$$

- *η is sub-additive:*

$$\eta(\mathbf{v}_1+\mathbf{v}_2) \leq \eta(\mathbf{v}_1)+\eta(\mathbf{v}_2) \qquad \textit{for all } \mathbf{v}_1,\mathbf{v}_2\in\mathbb{R}^d. \tag{14}$$

Proposition 2.9. *A convex function η is a variation entropy if and only if it is given by*

$$\eta = \eta(\nabla\phi) = \hat{\eta}(r,\boldsymbol{\theta}) = F(\boldsymbol{\theta})r, \tag{15}$$

where $F = F(\boldsymbol{\theta})$ is a scalar-valued function and where $c\in\mathbb{R}$ and r and $\boldsymbol{\theta}$ are the spherical polar coordinates of $\nabla\phi$. The convexity condition is in the 2-dimensional case:

$$F(\theta) + F''(\theta) \geq 0. \tag{16}$$

Remark 2.10. The convexity demand in three dimensions is more involved. We refer to [51] for details.

Proposition 2.11. *All semi-norms of $\nabla\phi$ are variation entropies.*

Corollary 2.12. *A direct consequence of the homogeneity property (12) in Theorem 2.8 is that the variation entropy flux is given by*

$$\mathbf{q} = \frac{\partial \mathbf{f}}{\partial \phi}\eta, \tag{17}$$

and that the variation entropy condition is thus rigorously understood as

$$\int_0^\infty \int_{\mathbb{R}^d} \eta \left(\partial_t v + \frac{\partial \mathbf{f}}{\partial \phi} \cdot \nabla v \right) \mathrm{d}\mathbf{x}\mathrm{d}t \geq 0, \tag{18}$$

for all test functions $v \in \mathcal{C}_c^\infty(\Omega \times (0, \infty)), v \geq 0$.

In the case of parabolic conservation laws we can write

$$\mathbf{q} = \frac{\partial \mathbf{f}}{\partial \phi}\eta + \frac{\partial \mathbf{f}}{\partial \nabla \phi}\nabla \eta. \tag{19}$$

Note that (17) is similar to the form of the compatibility condition of the classical entropy case when taking the derivative with respect to $\nabla \phi$:

$$\frac{\partial \mathbf{q}}{\partial \nabla \phi} = \frac{\partial \mathbf{f}}{\partial \phi} \otimes \frac{\partial \eta}{\partial \nabla \phi}. \tag{20}$$

Examples of variation entropies are

$$\eta = \eta(\nabla \phi) = \|\nabla \phi\|_2, \tag{21a}$$

$$\eta = \eta(\nabla \phi) = \mathbf{c} \cdot \nabla \phi, \text{ for } \mathbf{c} \in \mathbb{R}^d, \tag{21b}$$

$$\eta = \eta(\nabla \phi) = \|\nabla \phi\|_{\mathbf{A}} := \left(\nabla \phi^T \mathbf{A} \nabla \phi \right)^{1/2}, \text{ for positive semi-definite matrix } \mathbf{A}. \tag{21c}$$

where $\| \cdot \|_2$ is the standard 2-norm. Variation entropy (21b) is the only linear variation entropy.

Definition 2.13. *A pair of functions $(\eta, \mathbf{q})$ is called a variation entropy-variation entropy flux pair for the conservation law (7) if*

- *η is a variation entropy,*
- *the flux $\mathbf{q}$ is given by (17).*

Definition 2.14. *We call $\phi = \phi(\mathbf{x}, t)$ a variation entropy solution of (7) if ϕ is a weak solution and ϕ satisfies (8) in a weak sense for each variation entropy-variation entropy flux pair $(\eta, \mathbf{q})$.*

Physically relevant solutions are vanishing viscous solutions ϕ^ϵ satisfying:

$$\partial_t \phi^\epsilon + \nabla \cdot \mathbf{f}(\phi^\epsilon) = \epsilon \Delta \phi^\epsilon. \tag{22}$$

Suppose ϕ^ϵ is uniformly bounded in $L^\infty(\Omega)$ and

$$\phi^\epsilon \to \phi \quad \text{a.e. as} \quad \epsilon \to 0, \tag{23}$$

then we say that ϕ is a physically relevant solution. In the following theorem we state that physically relevant solutions are, apart from classical entropy solutions, also variation entropy solutions.

Theorem 2.15. *The limit solution $\phi = \lim_{\epsilon \to 0} \phi^\epsilon$ is a variation entropy solution.*

Proof. See [51]. □

Analogously to the classical entropy case, in absence of boundary conditions we can integrate over the domain Ω to get a dissipation of the overall variation entropy:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \eta(\nabla\phi)\mathrm{d}\Omega \leq 0 \Rightarrow \int_\Omega \eta(\nabla\phi(\mathbf{x},t))\ \mathrm{d}\Omega \leq \int_\Omega \eta(\nabla\phi_0(\mathbf{x}))\ \mathrm{d}\Omega, \quad \text{for all } t>0. \tag{24}$$

3. The VMS-variation entropy framework for discontinuity capturing methods

In this section we employ the variation entropy concepts within the variational multiscale framework to derive a class of discontinuity capturing methods.

3.1. Starting point

We take the point of view that a good numerical method solves the conservation law problem:

find $\phi : \Omega \times \mathcal{I} \rightarrow \mathbb{R}$ *such that*

$$\partial_t\phi + \nabla\cdot\mathbf{f} = 0, \qquad (\mathbf{x},t)\in\Omega\times\mathcal{I}, \tag{25a}$$

$$\phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \qquad \mathbf{x}\in\Omega, \tag{25b}$$

with smooth flux $\mathbf{f} = \mathbf{f}(\phi)$ and at the same time does not harm the variation entropy condition

$$\partial_t\eta + \nabla\cdot\mathbf{q} \leq 0, \tag{26}$$

for variation entropy η. In the remainder of this section we derive a multiscale framework which endeavors this.

Remark 3.1. Here we focus on hyperbolic conservation laws. We want to emphasize that changing to the parabolic case is a trivial execution. Furthermore, one can augment the conservation law with a non-zero source term.

We start off with the regularized conservation law:

find $\phi^\epsilon : \Omega \times \mathcal{I} \rightarrow \mathbb{R}$ *such that*

$$\partial_t\phi^\epsilon + \nabla\cdot\mathbf{f}(\phi^\epsilon) = \epsilon\Delta\phi^\epsilon, \qquad (\mathbf{x},t)\in\Omega\times\mathcal{I}, \tag{27a}$$

$$\phi^\epsilon(\mathbf{x},0) = \phi_0(\mathbf{x}), \qquad \mathbf{x}\in\Omega, \tag{27b}$$

with regularization parameter $\epsilon \geq 0$. The initial condition $\phi(\mathbf{x},0) = \phi_0(\mathbf{x}) \in L^\infty(\Omega)$ is assumed to have compact support. Note that the limit solution is a variation entropy solution (Theorem 2.15). The weak form of this problem is:

find $\phi^\epsilon \in \mathcal{W}$ *such that for all* $w \in \mathcal{W}$

$$(w, \partial_t\phi^\epsilon)_{L^2(\Omega)} - (\mathbf{f}(\phi^\epsilon), \nabla w)_{L^2(\Omega)} = -(\phi^\epsilon, w)_{\mathcal{W}}. \tag{28}$$

Here $(\cdot,\cdot)_{L^2(\Omega)}$ is the standard L^2-innerproduct and we have used the self-adjoint positive-definite linear viscosity operator to define an inner product:

$$(u,v)_{\mathcal{W}} := (\epsilon\nabla u, \nabla v)_{L^2(\Omega)}. \tag{29}$$

A natural norm is the *energy norm*:

$$\|v\|^2_{\mathcal{W}} := \left\|\epsilon^{1/2}\nabla v\right\|^2_{L^2(\Omega)}. \tag{30}$$

For more details about the construction of an energy norm we refer to [56].

3.2. *Mesh representation and geometrical mapping*

Let the parametric domain be $\hat{\Omega} := (-1,1)^d \subset \mathbb{R}^d$ and let us denote the mesh in the parametric domain with $\mathcal{M}$. The elements Q of $\mathcal{M}$ have element size $h_Q = \text{diag}(Q)$ (diagonal length). We denote the physical domain by $\Omega \subset \mathbb{R}^d$ and the continuously differentiable geometrical map (with continuously differentiable inverse) by $\mathbf{F} : \hat{\Omega} \to \Omega$. Each parametric element $Q \in \mathcal{M}$ maps into a physical element

$$\Omega_K = \mathbf{F}(Q), \tag{31}$$

which induces a physical mesh:

$$\mathcal{K} = \mathbf{F}(\mathcal{M}) := \{\Omega_K : \Omega_K = \mathbf{F}(Q), Q \in \mathcal{M}\}. \tag{32}$$

We denote the corresponding Jacobian by $\mathbf{J} = D\mathbf{F} = \partial \mathbf{x}/\partial \boldsymbol{\xi}$, or in index notation $J_{ij} = \partial x_i/\partial \xi_j$. We define the second-rank element metric tensor as

$$\mathbf{G} = \frac{\partial \boldsymbol{\xi}}{\partial \mathbf{x}}^T \frac{\partial \boldsymbol{\xi}}{\partial \mathbf{x}} = \mathbf{J}^{-T}\mathbf{J}^{-1}, \quad \text{or in index notation} \quad G_{ij} = \frac{\partial \xi_k}{\partial x_i}\frac{\partial \xi_k}{\partial x_j}. \tag{33}$$

The inverse is given by

$$\mathbf{G}^{-1} = \frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}}\frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}}^T = \mathbf{J}\mathbf{J}^T, \quad \text{with the index notation} \quad G_{ij}^{-1} = \frac{\partial x_i}{\partial \xi_k}\frac{\partial x_j}{\partial \xi_k}. \tag{34}$$

Furthermore we define the physical mesh size h_K as

$$h_K^2 = \frac{h_Q^2}{d}\|\mathbf{J}\|_F^2, \tag{35}$$

where the subscript F refers to the Frobenius norm given by

$$\|\mathbf{J}\|_F^2 = \sum_{i,j=1}^{d}\left(\frac{\partial x_i}{\partial \xi_j}\right)^2 = \text{Tr}(\mathbf{J}\mathbf{J}^T) = \text{Tr}(\mathbf{G}^{-1}), \tag{36}$$

with Tr the trace operator. The Frobenius norm is a natural choice for mesh metrics since it is rotation-invariant and appears in several well-known mesh quality measures. Another benefit is its lower computational costs compared to the standard p-norm [57]. Furthermore, on a Cartesian mesh it reduces to the length of the diagonal of an element. We use the notation $\nabla_{\boldsymbol{\xi}}$ to distinguish differentiation with respect to the reference coordinates $\boldsymbol{\xi}$ from the gradient in physical coordinates ∇.

On uniform Cartesian meshes we use the notation $\partial x/\partial \xi := \partial x_1/\partial \xi_1 = \partial x_2/\partial \xi_2 = \partial x_3/\partial \xi_3 > 0$.

3.3. *The multiscale split*

The residual-based variational multiscale approach splits the solution into a large-scale and a small-scale component. The large-scale component is solved numerically, whereas the small-scale contribution is treated in an approximate sense. Assume that there exists an idempotent (and possibly nonlinear) projector $\mathscr{P}^h : \mathcal{W} \to \mathcal{W}^h$. The trial solution and weighting function spaces split as

$$\mathcal{W} = \mathscr{P}^h\mathcal{W} \oplus (\mathscr{I} - \mathscr{P}^h)\mathcal{W} = \mathcal{W}^h \oplus \mathcal{W}', \tag{37}$$

where $\mathcal{W}^h$ is the coarse-scale linear subspace and $\mathcal{W}'$ is its infinite-dimensional complement. This allows us to decompose $\phi^\epsilon \in \mathcal{W}$ and $w \in \mathcal{W}$ as:

$$\phi^\epsilon = (\phi^\epsilon)^h + (\phi^\epsilon)' \quad \text{and} \quad w = w^h + w', \tag{38}$$

where $(\phi^\epsilon)^h = \mathscr{P}^h \phi^\epsilon$ and $w^h = \mathscr{P}^h w$. Because $\mathcal{W}^h$ is a subset of $\mathcal{W}$, (28) implies that for all $w^h \in \mathcal{W}^h$

$$\begin{aligned}&(w^h, \partial_t((\phi^\epsilon)^h + (\phi^\epsilon)'))_{L^2(\Omega)} - (\mathbf{f}((\phi^\epsilon)^h + (\phi^\epsilon)'), \nabla w^h)_{L^2(\Omega)} \\ &= -\left((\phi^\epsilon)^h + (\phi^\epsilon)', w^h\right)_{\mathcal{W}},\end{aligned} \tag{39}$$

regardless of the possible nonlinearity of $\mathscr{P}^h$. Take for the coarse-scale space $\mathcal{W}^h \subset H^1(\Omega)$. Sending $\epsilon \to 0$ in (39) and noting that due to

$$\left|\left((\phi^\epsilon)^h, w^h\right)_{\mathcal{W}}\right| \leq \|\, (\phi^\epsilon)^h \,\|_{\mathcal{W}} \|w^h\|_{\mathcal{W}} \to 0 \quad \text{as} \quad \epsilon \to 0, \tag{40}$$

we arrive at

$$(w^h, \partial_t(\phi^h + \phi'))_{L^2(\Omega)} - (\mathbf{f}(\phi^h + \phi'), \nabla w^h)_{L^2(\Omega)} = -\left(\phi', w^h\right)_{\mathcal{W}}, \tag{41}$$

for all $w^h \in \mathcal{W}^h$, with $\phi^h := \lim_{\epsilon\to 0} (\phi^\epsilon)^h$ and $\phi' := \lim_{\epsilon\to 0} (\phi^\epsilon)'$. Here we use an abuse of notation for the term on the right-hand side which is the limit of the small-scale regularization term. In contrast to the large-scale component, the small-scale term does not vanish in general due to the (possibly) unbounded gradient $\nabla\phi'$. Note that this weak formulation is still exact. However, the infinite-dimensionality of $\mathcal{W}'$ does not allow for a discrete implementation.

Let η be a positive-valued variation entropy function $\eta = \eta(\nabla\phi) : \mathbb{R}^d \to \mathbb{R}_+$ (and thus nonlinear, eliminating the linear variation entropy (21b)). We assume that $\eta(\nabla w) \in L^2(\Omega)\ \forall w \in \mathcal{W}$. The large-scale solution space associated with η is defined as

$$\mathcal{V}^h := \eta(\nabla\mathcal{W}^h), \tag{42}$$

with the elements

$$\eta^h := \eta(\nabla\phi^h) \in \mathcal{V}^h. \tag{43}$$

We define the small-scale variation entropy as $\eta' := \eta(\nabla\phi) - \eta^h$. Let us denote the residual of the conservation law and that of the variation entropy condition as:

$$\mathscr{R}_{\rm CL}\phi := \partial_t\phi + \nabla\cdot\mathbf{f}, \tag{44}$$

$$\begin{aligned}\mathscr{R}_{\rm VE}\eta &:= \partial_t\eta + \nabla\cdot\mathbf{q} \\ &= \frac{\partial\eta}{\partial\nabla\phi}\cdot\nabla\left(\mathscr{R}_{\rm CL}\phi\right).\end{aligned} \tag{45}$$

3.4. A standard optimality projector

To establish scale separation the projector $\mathscr{P}^h$ needs to be selected. We construct the projector via the minimization of a functional. The standard approach is the following. Consider the minimization problem:

find $\phi^h \in \mathcal{W}^h$ such that:

$$\mathscr{L}(\phi - \phi^h) = \inf_{\theta^h\in\mathcal{W}^h} \mathscr{L}(\phi - \theta^h) \tag{46}$$

where the quadratic functional is given by

$$\mathscr{L}(\phi) = \tfrac{1}{2}\|\phi\|^2_{\mathcal{W}}. \tag{47}$$

Lemma 3.2. *The functional $\mathscr{M} : \mathcal{W}^h \to \mathbb{R}$ given by*

$$\mathscr{M}(w^h) := \tfrac{1}{2}\|\phi - w^h\|^2_{\mathcal{W}} \tag{48}$$

is strictly convex.

Proof. This follows from the positive definiteness of the second derivative which equals

$$\mathrm{d}^2\mathscr{M}(w^h)(u^h, v^h) = (u^h, v^h)_{\mathcal{W}}, \tag{49}$$

for $u^h, v^h \in \mathcal{W}^h$. □

Theorem 3.3. *Assuming $\mathcal{W}^h$ is closed, problem (46)-(47) has a unique solution.*

Proof. This is a consequence of Lemma 3.2. See also [46]. □

The multiscale split projector (37) is now defined as:

$$\mathscr{P}^h\phi = \underset{\phi^h \in \mathcal{W}^h}{\arg\min}\, \mathscr{L}(\phi - \phi^h)\ . \tag{50}$$

We obtain a stationary point when the Gateaux derivative of the functional $\mathscr{L}$ in direction w^h vanishes:

$\mathscr{P}^h : \phi \in \mathcal{W} \to \phi^h \in \mathcal{W}^h$: *find $\phi^h \in \mathcal{W}^h$ such that for all $w^h \in \mathcal{W}^h$:*

$$\mathrm{d}\mathscr{L}(\phi - \phi^h)(w^h) = 0. \tag{51}$$

Evaluating (51), the multiscale split projector takes the form:

$\mathscr{P}^h : \phi \in \mathcal{W} \to \phi^h \in \mathcal{W}^h$: *find $\phi^h \in \mathcal{W}^h$ such that for all $w^h \in \mathcal{W}^h$:*

$$(w^h, \phi^h - \phi)_{\mathcal{W}} = 0. \tag{52}$$

Employing this relation in the VMS weak formulation, via the multiscale split (38), cancels the symmetric contributions on the small-scales:

$$(w^h, \phi')_{\mathcal{W}} = 0. \tag{53}$$

As a result, the small-scale solution space is given by

$$\mathcal{W}' = \left\{\phi' \in \mathcal{W} :\ (w^h, \phi')_{\mathcal{W}} = 0 \quad \text{for all } w^h \in \mathcal{W}^h\right\}. \tag{54}$$

Remark 3.4. The orthogonality (53) is linked to correct energy behavior for the convection-diffusion and the incompressible Navier-Stokes equations. For details we refer to [40, 58].

In the standard VMS framework the small-scales of the governing equations need to be modeled to arrive at a numerical method. For general details about small-scale modeling we refer to [37, 58, 59]. We employ the standard small-scale model for ϕ':

$$\hat{\phi}' = -\,\tau_{\mathrm{CL}}\mathscr{R}_{\mathrm{CL}}\phi^h, \tag{55a}$$
$$\partial_t\hat{\phi}' = 0, \tag{55b}$$

The scalar stabilization parameter τ_{CL} is a mesh-dependent approximation (based on inverse estimates, see e.g [60]) of the inverse of the differential operator. We use the hat-sign to indicate that (55) is a small-scale model instead of it being the actual small-scales. In the following we use this approximation and ignore the hat-sign. The current approach is known as the concept of static small-scales, due to assumption (55b). We note that, as an alternative, one can employ dynamic small-scales. In that case a dynamic version of (55a) is used and the second modeling assumption, relation (55b), is not made. This dynamic approach has some advantages [40, 58, 61]. Furthermore, we remark that nonlinear contributions of the small-scales can be incorporated in the residual, see e.g. [37].

By employing the orthogonality (53) and the small-scale model (55) in an SUPG fashion in (39) we arrive at:

find $\phi^h \in \mathcal{W}^h$ *such that for all* $w^h \in \mathcal{W}^h$

$$(w^h, \partial_t \phi^h)_{L^2(\Omega)} - (\nabla \mathbf{w}^h, \mathbf{f}(\phi^h))_{L^2(\Omega)} + \sum_K ((\tau_{\text{CL}})_K \frac{\partial \mathbf{f}}{\partial \phi^h} \cdot \nabla w^h, \mathscr{R}_{CL}(\phi^h)))_{L^2(\Omega_K)} = 0. \tag{56}$$

The consequence is thus that both the large and small-scale components stemming from the regularized term vanish. However, when incorporating the variation entropy condition in the projector the small-scale contribution does not vanish. We present this approach in the next subsection.

3.5. A variation entropy optimality projector

Here we present a new optimality projector that uses the variation entropy condition. This naturally leads to a discontinuity capturing term.

Remark 3.5. Here we choose to enforces the variation entropy condition in an indirect manner. As an alternative one could use a more direct approach. We present the corresponding steps in Appendix A. This alternative approach does not provide a convex problem and as such uniqueness of the minimization problem can not be guaranteed.

Consider the minimization problem:

find $\phi^h \in \mathcal{W}^h$ *such that:*

$$\mathscr{L}(\phi - \phi^h) = \inf_{\theta^h \in \mathcal{K}^h} \mathscr{L}(\phi - \theta^h), \tag{57}$$

where the constraint set reads:

$$\mathcal{K}^h := \left\{ \phi^h \in \mathcal{W}^h : \ (v^h, \eta(\nabla \phi^h) - \eta(\nabla \phi))_{L^2(\Omega)} \leq 0 \quad \text{for all } v^h \in \mathcal{V}^h \right\}. \tag{58}$$

Lemma 3.6. *The solution space* $\mathcal{K}^h$ *is convex.*

Proof. This is direct consequence of the sub-additivity and the homogeneity of the variation entropy. Indeed let $0 \leq \zeta \leq 1$ and let $\phi_1^h, \phi_2^h \in \mathcal{K}^h$ then

$$\begin{aligned}
&(v^h, \eta(\zeta \nabla \phi_1^h + (1-\zeta)\nabla \phi_2^h))_{L^2(\Omega)} && (59)\\
&\leq (v^h, \eta(\zeta \nabla \phi_1^h) + \eta((1-\zeta)\nabla \phi_2^h))_{L^2(\Omega)} \quad && \textit{(sub-additivity)}\\
&\leq (v^h, \zeta\eta(\nabla \phi_1^h) + (1-\zeta)\eta(\nabla \phi_2^h))_{L^2(\Omega)} \quad && \textit{(homogeneity)}\\
&\leq (v^h, \zeta\eta(\nabla \phi) + (1-\zeta)\eta(\nabla \phi))_{L^2(\Omega)} \quad && (\phi_1^h, \phi_2^h \in \mathcal{K}^h)\\
&= (v^h, \eta(\nabla \phi))_{L^2(\Omega)}, && (60)
\end{aligned}$$

for all $v^h \in \mathcal{V}^h$. This implies $\zeta\phi_1^h + (1-\zeta)\phi_2^h \in \mathcal{K}^h$. □

Theorem 3.7. *Problem (57)-(58) has a unique solution.*

Proof. The constraint set $\mathcal{K}^h$ is convex. Uniqueness follows from Lemma 3.2 in a similar fashion as in Theorem 3.3. Details can be found in [46]. □

We proceed by opening the solution space. We penalize violating the constraint defined in (58). The constraint problem (57)-(58) converts into the unconstrained minimization problem:

find $\phi^h \in \mathcal{W}^h$ *such that:*

$$\mathscr{J}(\phi-\phi^h,\phi,\phi^h) = \inf_{\theta^h\in\mathcal{W}^h} \mathscr{J}(\phi-\theta^h,\phi,\theta^h), \tag{61a}$$

where we have defined the functional $\mathscr{J}:\mathcal{W}'\times\mathcal{W}\times\mathcal{W}^h \to \mathbb{R}$ *as*

$$\mathscr{J}(w_1,w_2,w_3) = \mathscr{L}(w_1) + \frac{1}{2}\|\sqrt{\mu}\,\{\eta(\nabla w_2)-\eta(\nabla w_3)\}_-\,\|^2_{L^2(\Omega)}. \tag{61b}$$

where $\{\cdot\}_-$, defined as $\{a\}_- = (a-|a|)/2$, isolates the negative part of its argument. Here $\mu=\mu(\Omega)\geq 0$ is a parameter penalizing excess variation entropy of the coarse scale solution. The unit of μ is $[\mu] = [\phi]^2/([\eta]^2T)$[1]. In the case that the unit of η is that of the solution over length, i.e. $[\eta]=[\phi]/L$, μ has the unit of a viscosity: $[\mu]=L^2/T$.

Proposition 3.8. *The functional* $\mathscr{J}=\mathscr{J}(\phi-\phi^h,\phi,\phi^h)$ *is bounded:*

$$\mathscr{L}(\phi-\phi^h) \leq \mathscr{J}(\phi-\phi^h,\phi,\phi^h) \leq \mathscr{J}_{\rm up}(\phi-\phi^h) \tag{62a}$$

where the upper bound is given by

$$\mathscr{J}_{\rm up}(\phi-\phi^h) = \mathscr{L}(\phi-\phi^h) + \frac{1}{2}\|\sqrt{\mu}\eta(\nabla(\phi-\phi^h))\|^2_{L^2(\Omega)}. \tag{62b}$$

Proof. This follows from the sub-additivity of η (14):

$$\begin{aligned}\eta(\nabla\phi)-\eta^h =& \eta(\nabla\phi)-\eta(\nabla\phi+(\nabla\phi^h-\nabla\phi))\\ \geq& \eta(\nabla\phi)-\eta(\nabla\phi)-\eta(\nabla\phi^h-\nabla\phi)\\ =& -\eta(\nabla\phi^h-\nabla\phi).\end{aligned} \tag{63}$$

□

Remark 3.9. In the case that the variation entropy equals $\eta=\|\nabla\phi\|_2$, the upper bound converts into

$$\begin{aligned}\mathscr{J}_{\rm up}(\phi-\phi^h) &= \frac{1}{2}\|\phi-\phi^h\|^2_{\mathcal{W}} + \frac{1}{2}\|\mu^{1/2}\nabla(\phi-\phi^h)\|^2_{L^2(\Omega)}\\ &= \frac{1}{2}\|(\epsilon+\mu)^{1/2}\nabla(\phi-\phi^h)\|^2_{L^2(\Omega)},\end{aligned} \tag{64}$$

which is the energy norm with viscosity $\epsilon+\mu$.

We penalize violating the constraint defined in (58) by defining the projector $\mathscr{P}^h\phi:\mathcal{W}\to\mathcal{W}^h$ as:

$$\mathscr{P}^h\phi = \underset{\phi^h\in\mathcal{W}^h}{\arg\min}\, \mathscr{J}(\phi-\phi^h,\phi,\phi^h)\ . \tag{65}$$

Remark 3.10. This can be viewed as a nonlinear Tikhonov-like regularization of orthogonal projection in $\mathcal{W}$. Alternatively, it can be seen as a penalty regularization of the inequality-constrained projection

$$\mathscr{P}^h_{\rm c}\phi = \arg\left\{\begin{array}{l}\displaystyle\min_{\phi^h\in\mathcal{W}^h} \mathscr{L}(\phi-\phi^h)\\[2ex] \text{subject to}\ \ \eta\left(\nabla\phi^h\right)\leq\eta(\nabla\phi)\ \text{a.e. in}\ \Omega\end{array}\right\}. \tag{66}$$

[1]In this paper we use the notation $[a]$ to denote the unit of quantity a. Furthermore, L denotes and length unit and T a time unit.

The first-order optimality conditions for $\mathscr{P}^h$ follow from equating the Gateaux derivative in direction w^h to zero. Noting that

$$\mathrm{d}\ \eta(\nabla\phi^h)(\nabla w^h) = \frac{\partial\eta}{\partial\nabla\phi^h}\cdot\nabla w^h, \tag{67}$$

we obtain the problem:

$\mathscr{P}^h : \phi \in \mathcal{W} \to \phi^h \in \mathcal{W}^h$: *find* $\phi^h \in \mathcal{W}^h$ *such that for all* $w^h \in \mathcal{W}^h$:

$$\left(\phi', w^h\right)_{\mathcal{W}} = -\left(\mu\{\eta'\}_-\frac{\partial\eta^h}{\partial\nabla\phi^h}, \nabla w^h\right)_{L^2(\Omega)} . \tag{68}$$

Using the homogeneity of η^h, i.e. relation (12), we can write:

$$\frac{\partial\eta}{\partial\nabla\phi^h} = \frac{1}{\eta^h}\left(\frac{\partial\eta^h}{\partial\nabla\phi^h}\otimes\frac{\partial\eta^h}{\partial\nabla\phi^h}\right)\nabla\phi^h. \tag{69}$$

Thus we arrive at

$$\left(\phi', w^h\right)_{\mathcal{W}} = \left(\mathbf{K}\nabla\phi^h, \nabla w^h\right)_{L^2(\Omega)} , \tag{70}$$

in which the matrix $\mathbf{K}$ is given by:

$$\mathbf{K} = \nu\left(\frac{\partial\eta^h}{\partial\nabla\phi^h}\otimes\frac{\partial\eta^h}{\partial\nabla\phi^h}\right) , \tag{71a}$$

$$\nu = -\mu\frac{\{\eta'\}_-}{\eta^h} . \tag{71b}$$

The parameter $\nu \geq 0$, referred to as *variation entropy viscosity*, scales with the relative error of the variation entropy η^h and has unit $[\nu] = [\mu] = [\phi]^2[\eta]^{-2}T^{-1}$. Note that $\mathbf{K}$ has the unit of a viscosity:

$$[\mathbf{K}] = [\nu]\frac{[\eta]^2}{[\nabla\phi]^2} = \frac{L^2}{T}. \tag{72}$$

The matrix (71a) acts as *diffusion based on the variation entropy residual*. Note that the diffusion operator of the streamline upwind method [12] acts in the direction of the flow. For discontinuity capturing control of gradients in the direction $\nabla\phi^h$ is relevant [15]. The diffusion operator $\mathbf{K}$ acts in the direction $\partial\eta/\partial\nabla\phi^h$. This is the direction in which the variation entropy changes and is thus a natural direction to add diffusion.

Lemma 3.11. *The matrix* $\mathbf{K}$ *is symmetric positive semi-definite.*

Proof. Symmetry is trivial and the positive semi-definiteness is a direct consequence of ν being positive. ☐

Remark 3.12. One could alternatively start from the constrained projector $\mathscr{P}^h_{\mathrm{c}}$ and approximate the Lagrange multiplier associated with the constraint by penalizing $-\mu\{\eta'\}_-$ to obtain the same result.

At this point, no approximation has been made. We may substitute (70)-(71) into (41), illustrating how unresolved viscous dissipation in the fine-scale solution is expressed in terms of variation entropy in the coarse-scale problem when the coarse scales are defined by the nonlinear projector $\mathscr{P}^h$. Notice that, when taking the limit $\epsilon \to 0$ the right-hand side of (71) does not vanish in this limit. This is consistent with the necessity of shock-capturing operators in the inviscid limit. Further, the right-hand side of (71) is independent of the precise choice of viscous operator, as one would hope in the case that an arbitrary regularization introduced for analysis purposes.

3.6. *Small-scale model variation entropy*

The current VMS-VE framework requires a model for the negative part of the small-scale variation entropy $\{\eta'\}_-$. This opens the door to explore several small-scale models leading to different numerical methods. Note that the small-scale variation entropy $\eta' = \eta(\nabla\phi) - \eta^h$ is linked to the small-scale solution ϕ' via:

$$\begin{aligned}\{\eta'\}_- &= \{\eta(\nabla\phi) - \eta^h\}_- \\ &= \{\eta(\nabla\phi^h + \nabla\phi') - \eta^h\}_- \\ &\leq \{\eta(\nabla\phi')\}_- \\ &= 0.\end{aligned} \tag{73}$$

Thus employing the model $\{\eta'\}_- = \{\eta(\nabla\phi')\}_-$ where the small-scale solution ϕ' is determined by the standard static model (55) causes the discontinuity capturing operator to vanish.

We propose a model for $\{\eta'\}_-$ inspired by the variation entropy condition. Other possibilities may lead to an improved method with practical benefits and/or theoretical advantages. Remark that in the case of smooth solutions the variation entropy condition converts into an equality. Here we use the standard VMS method and write down the Euler-Lagrange equations of small-scale equation. Following this reasoning we propose the model for $\{\eta'\}_-$:

$$\widehat{\{\eta'\}_-}_{\mathrm{VE}} = -\tau_{\mathrm{VE}} \left\{\mathscr{R}_{\mathrm{VE}}\left(\eta^h\right)\right\}_+ , \tag{74}$$

where the hat-symbol indicates the modeling step. Here $\tau_{\mathrm{VE}} \geq 0$ represents a time-scale associated with the variation entropy. We note that τ_{VE} is an element-wise parameter: $\tau_{\mathrm{VE}} = (\tau_{\mathrm{VE}})_K$. We wish to emphasize that model (74) is residual-based, both directly with residual $\mathscr{R}_{\mathrm{VE}}$ and with residual $\mathscr{R}_{\mathrm{CL}}$, see (45).

3.7. *Variation entropy viscosity*

The variation entropy viscosity corresponding to the model (74) is:

$$\nu_{\mathrm{VE}} = \mu\ \tau_{\mathrm{VE}} \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\eta^h\right)\right\}_+}{\eta^h} , \tag{75}$$

where the subscript VE refers to the variation-entropy residual. Despite the fact that the variation entropy viscosities are element-wise parameters, for the ease of notation we do not explicitly write a subscript K referring to element K in this subsection. Note that the variation entropy viscosity (75) vanishes when the variation entropy condition is satisfied.

The product $\mu\ \tau_{\mathrm{VE}}$ needs to be modeled. A natural approach would be to model the terms separately. In this case, a standard VMS approach could be used to model the intrinsic time-scale associated with the variation entropy, τ_{VE}, i.e. one could use a discrete approximation of the inverse of the corresponding differential operator[2]. The term μ is a penalty parameter that links the variation entropy to the regularization term. Recall that the unit of μ is $[\phi]^2[\eta]^{-2}T^{-1}$. Since μ is associated with the variation entropy, a natural choice for the time-scale in μ is τ_{VE}^{-1}. Following this approach, the model for τ_{VE} would cancel in the product $\mu\ \tau_{\mathrm{VE}}$. This suggests the alternative to model the product $\mu\ \tau_{\mathrm{VE}}$ as one quantity instead of modeling the separate terms. This is how we proceed. As μ connects the variation entropy to the regularization term associated with the conservation law and this connection is governed by the operator $\partial\eta/\partial\nabla\phi \cdot \nabla$ (see (45)), we employ this operator to determine the product $\mu\ \tau_{\mathrm{VE}}$. By applying the chain rule this operator may be

[2] In the linear convection-diffusion case one could use $\tau_{\mathrm{VE}} = \tau_{\mathrm{CL}}$ as the differential operators equal (see (105) in Section 3.10).

written as:

$$\frac{\partial \eta^h}{\partial \nabla \phi^h} \cdot \nabla = \left(\frac{\partial \boldsymbol{\xi}}{\partial \mathbf{x}} \frac{\partial \eta^h}{\partial \nabla \phi^h} \right) \frac{\partial}{\partial \boldsymbol{\xi}} \\ = \left(\mathbf{J}^{-1} \frac{\partial \eta^h}{\partial \nabla \phi^h} \right) \frac{\partial}{\partial \boldsymbol{\xi}}. \tag{76}$$

Note that the unit of the product $\mu\ \tau_{\mathrm{VE}}$ is the inverse square of that of the operator $\partial\eta/\partial\nabla\phi \cdot \nabla$ (the units are $[\phi]^2[\eta]^{-2}$ and $[\phi]^{-1}[\eta]$ respectively). We propose to use the discrete approximation of the inverse square of the operator $\partial\eta/\partial\nabla\phi \cdot \nabla$ as a model for $\mu\ \tau_{\mathrm{VE}}$. We take:

$$\mu\ \tau_{\mathrm{VE}} = C\ h_Q^2 \left|\left|\left| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right|\right|\right|_{\mathbf{G}}^{-2}, \tag{77}$$

where C is some unitless constant. Remark that a similar approximation technique also employing reference coordinates has been used to derive the stabilization parameter τ_{CL}, see e.g. [37]. The variation entropy viscosity thus converts into

$$\nu_{\mathrm{VE}} = C\ h_Q^2 \left|\left|\left| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right|\right|\right|_{\mathbf{G}}^{-2} \frac{\left\{ \mathscr{R}_{\mathrm{VE}} \left(\eta^h \right) \right\}_+}{\eta^h}\ . \tag{78}$$

Remark 3.13. Viscosity coefficients are usually determined via introducing a shock-capturing quantity and a length-scale. In the small-scale model (74) the quantity $\left\{ \mathscr{R}_{\mathrm{VE}} \left(\eta^h \right) \right\}_+ / \eta^h$ serves as shock-capturing quantity (and has unit T^{-1}).

The next step is to select a variation entropy. We propose two options. The simplest choice for the variation entropy is to take $\eta^h = \|\nabla\phi^h\|_2$. Remark that this variation entropy is objective, see [51]. The corresponding variation entropy viscosity takes the form:

$$\eta^h = \|\nabla \phi^h\|_2 \quad \Rightarrow \quad \nu_{\mathrm{VE}} = C\ h_Q^2 \left(\frac{\|\nabla \phi^h\|_2}{|||\nabla \phi^h|||_{\mathbf{G}}} \right) \frac{\left\{ \mathscr{R}_{\mathrm{VE}} \left(\|\nabla \phi^h\|_2 \right) \right\}_+}{|||\nabla \phi^h|||_{\mathbf{G}}}\ . \tag{79}$$

Another option is to select $\eta = \left|\left|\left| \nabla \phi^h \right|\right|\right|_{\mathbf{A}}$ which is defined for a positive semi-definite symmetric matrix as $|||\nabla\phi|||_{\mathbf{A}}^2 := \nabla\phi^T \mathbf{A} \nabla\phi$, see (21c). This is indeed a variation entropy and is rotation invariant whenever

$$\mathbf{A}(\mathbf{R}\mathbf{x}) = \mathbf{R}\mathbf{A}(\mathbf{x})\mathbf{R}^T \tag{80}$$

for rotation matrix $\mathbf{R}$, see [51]. We suggest to take $\mathbf{A} = \mathbf{G}^{-1}$, i.e. $\eta^h = \left|\left|\left| \nabla \phi^h \right|\right|\right|_{\mathbf{G}^{-1}} = \|\nabla_{\boldsymbol{\xi}} \phi^h\|_2$. Trivially $\mathbf{G}^{-1} = \mathbf{G}^{-1}(\mathbf{x})$ satisfies (80). The variation entropy viscosity corresponding to this choice is:

$$\eta^h = \|\nabla_{\boldsymbol{\xi}} \phi^h\|_2 \quad \Rightarrow \quad \nu_{\mathrm{VE}} = C\ h_Q^2 \frac{\left\{ \mathscr{R}_{\mathrm{VE}} \left(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2 \right) \right\}_+}{\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2}\ . \tag{81}$$

Proposition 3.14. *On an uniform Cartesian mesh there holds on element K:*

$$\mathbf{G}_K^{-1} = \mathbf{J}_K \mathbf{J}_K^T = \left(\frac{\partial x}{\partial \xi}\right)^2 \mathbf{I}_K, \tag{82a}$$

$$h_K^2 = \frac{h_Q^2}{d} \|\mathbf{J}_K\|_F^2 = h_Q^2 \left(\frac{\partial x}{\partial \xi}\right)^2, \tag{82b}$$

$$\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2 = \left\|\left|\nabla \phi^h\right|\right\|_{\mathbf{G}_K^{-1}} = \|\nabla \phi^h\|_2 \frac{\partial x}{\partial \xi}, \tag{82c}$$

$$\left\|\left|\nabla \phi^h\right|\right\|_{\mathbf{G}} = \|\nabla \phi^h\|_2 \frac{\partial \xi}{\partial x}. \tag{82d}$$

Lemma 3.15. *On uniform Cartesian quadratic/cubic meshes we have*

$$\nu_{VE}\left(\|\nabla \phi^h\|_2\right) = C\ h_K^2 \frac{\left\{\mathscr{R}_{VE}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2}, \tag{83a}$$

$$\nu_{VE}\left(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2\right) = C\ h_Q^2 \frac{\left\{\mathscr{R}_{VE}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2}, \tag{83b}$$

Proof. Using (82b) and (82d) the first identity is obtained:

$$\begin{aligned}
\nu_{\mathrm{VE}}(\|\nabla \phi^h\|_2) &= C\ h_Q^2 \left(\frac{\|\nabla \phi^h\|_2}{\|\!|\nabla \phi^h|\!\|_{\mathbf{G}}}\right)^2 \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2} \\
&= C\ h_Q^2 \left(\frac{\partial x}{\partial \xi}\right)^2 \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2} \\
&= C\ h_K^2 \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2},
\end{aligned} \tag{84}$$

The second expression follows via (45), (82a) and (82c):

$$\begin{aligned}
\nu_{\mathrm{VE}}(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2) &= C\ h_Q^2 \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2\right)\right\}_+}{\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2} \\
&= C\ h_Q^2 \frac{\left\{\dfrac{\mathbf{G}^{-1}\nabla \phi^h}{\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2} \cdot \nabla(\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right))\right\}_+}{\|\nabla \phi^h\|_2 \partial x/\partial \xi} \\
&= C\ h_Q^2 \frac{\left\{\dfrac{(\partial x/\partial \xi)^2\, \nabla \phi^h}{\|\nabla \phi^h\|_2 \partial x/\partial \xi} \cdot \nabla(\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right))\right\}_+}{\|\nabla \phi^h\|_2 \partial x/\partial \xi} \\
&= C\ h_Q^2 \frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla \phi^h\|_2\right)\right\}_+}{\|\nabla \phi^h\|_2}.
\end{aligned} \tag{85}$$

□

Corollary 3.16. *On uniform Cartesian quadratic/cubic meshes we have the identity:*

$$\nu_{VE}\left(\|\nabla \phi^h\|_2\right) = \left(\frac{\partial x}{\partial \xi}\right)^2 \nu_{VE}\left(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_2\right). \tag{86}$$

To avoid singularities we introduce a regularized variation entropy η_ε^h, see also [51]. Let us define the regularization of variation entropy $\left|\left|\left|\nabla\phi^h\right|\right|\right|_{\mathbf{A}}$ for regularization parameter $0 < \varepsilon \ll 1$ via:

$$\left(\eta^h_\varepsilon\right)^2 = \left|\left|\left|\nabla\phi^h\right|\right|\right|^2_{\varepsilon,\mathbf{A}} := \left|\left|\left|\nabla\phi^h\right|\right|\right|^2_{\mathbf{A}} + \varepsilon^2\frac{\mathrm{Tr}(\mathbf{A})}{d}. \tag{87}$$

Furthermore we also define:

$$\|\nabla\phi\|^2_{\varepsilon,2} := \|\nabla\phi\|^2_2 + \varepsilon^2. \tag{88}$$

The resulting expressions for the variation entropies chosen above are

$$\eta^h = \|\nabla\phi^h\|_2 \quad \Rightarrow \quad \left(\eta^h_\varepsilon\right)^2 = \|\nabla\phi^h\|^2_{\varepsilon,2}\ , \tag{89a}$$

$$\eta^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_2 \quad \Rightarrow \quad \left(\eta^h_\varepsilon\right)^2 = \left|\left|\left|\nabla\phi^h\right|\right|\right|^2_{\varepsilon,\mathbf{G}^{-1}} = \|\nabla_{\boldsymbol{\xi}}\phi^h\|^2_2 + \varepsilon^2\|\mathbf{J}\|^2_F/d =: \|\nabla_{\boldsymbol{\xi}}\phi^h\|^2_{\varepsilon_\xi,2}\ , \tag{89b}$$

where the regularization parameters are related as

$$\varepsilon^2_\xi = \varepsilon^2\|\mathbf{J}\|^2_F/d. \tag{90}$$

We apply the regularization both to the shock-capturing quantities and the prefactors yielding the following regularized variation entropy viscosities:

$$\eta^h_\varepsilon = \|\nabla\phi^h\|_{\varepsilon,2} \quad \Rightarrow \quad \nu_{\mathrm{VE}} = C\ h^2_Q\left(\frac{\|\nabla\phi^h\|_{\varepsilon,2}}{\left|\left|\left|\nabla\phi^h\right|\right|\right|_{\varepsilon,\mathbf{G}}}\right)\frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla\phi^h\|_{\varepsilon,2}\right)\right\}_+}{\left|\left|\left|\nabla\phi^h\right|\right|\right|_{\varepsilon,\mathbf{G}}}\ , \tag{91a}$$

$$\eta^h_\varepsilon = \|\nabla_{\boldsymbol{\xi}}\phi^h\|^2_{\varepsilon_\xi,2} \quad \Rightarrow \quad \nu_{\mathrm{VE}} = \ C\ h^2_Q\frac{\left\{\mathscr{R}_{\mathrm{VE}}\left(\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}\right)\right\}_+}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}}\ . \tag{91b}$$

Remark 3.17. Applying solely regularization in (78) to derive regularized versions of the expressions (79) and (81) does not exclude singularities.

The specific regularization choice ensures that Corollary 3.16 also holds in the regularized case.

Corollary 3.18. *On uniform Cartesian quadratic/cubic meshes we have the identity:*

$$\nu_{VE}\ \left(\|\nabla\phi^h\|_{\varepsilon,2}\right) = \left(\frac{\partial x}{\partial\xi}\right)^2\nu_{VE}\ \left(\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}\right), \tag{92}$$

where the terms in the brackets after ν_{VE} refer to (91a) and (91b) respectively.

3.8. Diffusion matrices

Let us first consider the case $\eta^h_\varepsilon = \|\nabla\phi^h\|_{\varepsilon,2}$. We use the non-regularized $\eta^h = \|\nabla\phi^h\|_2$ to derive the diffusion matrix and find via (71):

$$\mathbf{K}_K = (\nu_{\mathrm{VE}})_K\frac{\nabla\phi^h}{\|\nabla\phi^h\|_2}\otimes\frac{\nabla\phi^h}{\|\nabla\phi^h\|_2} \tag{93}$$

with variation entropy $(\nu_{\mathrm{VE}})_K$ given in (91a). Using the relation (70) we see that in this case the matrix $\mathbf{K}_K$ results in isotropic diffusion:

$$\left(\nabla w^h, \mathbf{K}_K\nabla\phi^h\right)_{L^2(\Omega_K)} = \left(\nabla w^h, (\nu_{\mathrm{VE}})_K\nabla\phi^h\right)_{L^2(\Omega_K)}. \tag{94}$$

In the other situation, i.e. $\eta_\varepsilon^h = \|\nabla_{\boldsymbol{\xi}} \phi^h\|_{\varepsilon_\xi,2}$, using also the corresponding non-regularized variation entropy yields for the diffusion matrix:

$$\mathbf{K}_K = (\nu_{\text{VE}})_K \frac{\mathbf{G}^{-1}\nabla\phi^h}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2} \otimes \frac{\mathbf{G}^{-1}\nabla\phi^h}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2}. \tag{95}$$

with variation entropy $(\nu_{\text{VE}})_K$ given in (91b). The resulting diffusion contribution in the weak form is based on local gradients:

$$\begin{aligned}\left(\nabla w^h, \mathbf{K}_K \nabla \phi^h\right)_{L^2(\Omega_K)} &= \left(\nabla w^h, (\nu_{\text{VE}})_K \ \frac{\mathbf{J}\nabla_{\boldsymbol{\xi}}\phi^h}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2}\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2\right)_{L^2(\Omega_K)} \\ &= \left(\nabla_{\boldsymbol{\xi}} w^h, (\nu_{\text{VE}})_K \ \nabla_{\boldsymbol{\xi}}\phi^h\right)_{L^2(\Omega_K)}. \end{aligned} \tag{96}$$

Remark 3.19. We note that Guermond and Nazarov [62] use reference coordinates to enforce the maximum principle. They observe that local reference coordinates can provide more control over the gradients.

Theorem 3.20. *On uniform Cartesian quadratic/cubic meshes the choices $\eta = \|\nabla\phi\|_{\varepsilon,2}$ and $\eta = \|\nabla_{\boldsymbol{\xi}}\phi\|_{\varepsilon_\xi,2}$ coincide.*

Proof. This is a direct consequence of Corollary 3.18:

$$\begin{aligned}\left(\nabla_{\boldsymbol{\xi}} w^h, (\nu_{\text{VE}})_K \ (\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}) \ \nabla_{\boldsymbol{\xi}}\phi^h\right)_{L^2(\Omega_K)} &= \left(\nabla w^h, (\nu_{\text{VE}})_K \ (\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}) \ \left(\frac{\partial x}{\partial \xi}\right)^2 \ \nabla\phi^h\right)_{L^2(\Omega_K)} \\ &= \left(\nabla w^h, (\nu_{\text{VE}})_K \ (\|\nabla\phi^h\|_{\varepsilon,2}) \ \nabla\phi^h\right)_{L^2(\Omega_K)}. \end{aligned} \tag{97}$$

□

3.9. Complete semi-discrete formulations

By substituting the diffusion terms (94) and (96) with corresponding variation entropy viscosities (91) into (70) and using the SUPG model of (56) in (39), we arrive at the following variational formulation:

find $\phi^h \in \mathcal{W}^h$ such that for all $w^h \in \mathcal{W}^h$:

$$\begin{aligned}&\underbrace{\left(w^h, \partial_t\phi^h\right)_{L^2(\Omega)} - \left(\nabla w^h, \mathbf{f}\left(\phi^h\right)\right)_{L^2(\Omega)}}_{\text{Galerkin}} + \underbrace{\sum_K \left((\tau_{\text{CL}})_K \frac{\partial \mathbf{f}}{\partial \phi^h}\cdot\nabla w^h, \mathscr{R}_{CL}(\phi^h)\right)_{L^2(\Omega_K)}}_{\text{Stabilization}} \\ &+ \left\{\begin{array}{ll} \underbrace{\sum_K (\nabla w^h, (\nu_{\text{VE}})_K \nabla\phi^h)_{L^2(\Omega_K)}}_{\substack{\text{Discontinuity capturing}\\ \text{in physical coordinates}}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla\phi^h\|_{\varepsilon,2} \\ \underbrace{\sum_K (\nabla_{\boldsymbol{\xi}} w^h, (\nu_{\text{VE}})_K \nabla_{\boldsymbol{\xi}}\phi^h)_{L^2(\Omega_K)}}_{\substack{\text{Discontinuity capturing}\\ \text{in reference coordinates}}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2} \end{array}\right\} = 0 \end{aligned} \tag{98a}$$

where the variation entropy viscosity is:

$$\nu_{\mathrm{VE}} = \begin{cases} C\ h_Q^2 \left(\dfrac{\|\nabla \phi^h\|_{\varepsilon,2}}{\|\nabla \phi^h\|_{\varepsilon,\mathbf{G}}} \right) \dfrac{\left\{ \mathscr{R}_{\mathrm{VE}} \left(\|\nabla \phi^h\|_{\varepsilon,2} \right) \right\}_+}{\|\nabla \phi^h\|_{\varepsilon,\mathbf{G}}} & \text{if} \quad \eta_\varepsilon^h = \|\nabla \phi^h\|_{\varepsilon,2} \\ C\ h_Q^2 \dfrac{\left\{ \mathscr{R}_{\mathrm{VE}} \left(\|\nabla_{\boldsymbol{\xi}} \phi^h\|_{\varepsilon_\xi,2} \right) \right\}_+}{\|\nabla_{\boldsymbol{\xi}} \phi^h\|_{\varepsilon_\xi,2}} & \text{if} \quad \eta_\varepsilon^h = \|\nabla_{\boldsymbol{\xi}} \phi^h\|_{\varepsilon_\xi,2}. \end{cases} \tag{98b}$$

We conclude that the variation entropy optimality projector with the proper modeling choices *naturally* augments the VMS method with a discontinuity capturing term:

$$\boxed{\mathrm{VMS} + \mathrm{VE} \rightsquigarrow \mathrm{DC}} \tag{99}$$

This proves the conjecture of Bazilevs et al. [24]:

'the multiscale frame-work with a proper set of optimality conditions is the right underlying theoretical structure that may more naturally lead to discontinuity capturing formulations.'

Remark 3.21. It is possible to set a maximum to the introduced viscosity, see e.g. [48]. Based on first-order upwind techniques (which yields in some cases a monotone method) a natural choice would be to take the maximum viscosity as:

$$\nu_{\max} = C_{\max} h_K \left\| \frac{\partial \mathbf{f}}{\partial \phi} \right\|_2, \tag{100}$$

where $C_{\max}$ is some constant.

3.10. The convection-diffusion problem

In the preceding part of this section we have solely focused on the hyperbolic case. As claimed, the parabolic case is a straightforward extension, which we demonstrate here using the convection-diffusion model problem.

Let $\phi_0 = \phi_0(\mathbf{x})$, divergence-free velocity field $\mathbf{a} = \mathbf{a}(\phi)$ and diffusivity $\kappa \geq 0$ be given. The problem reads:

find $\phi = \phi(\mathbf{x}, t) : \Omega \times \mathbb{R}^+ \to \mathbb{R}$ such that:

$$\partial_t \phi + \mathbf{a} \cdot \nabla \phi - \kappa \Delta \phi = 0 \qquad \text{in } \Omega \times \mathcal{I}, \tag{101a}$$

$$\phi = g \qquad \text{on } \partial\Omega, \tag{101b}$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}) \quad \text{in } \Omega. \tag{101c}$$

The standard weak formulation is:

find $\phi \in H_g^1(\Omega)$ such that for all $w \in H_0^1(\Omega)$:

$$(w, \partial_t \phi + \mathbf{a} \cdot \nabla \phi)_{L^2(\Omega)} + (\nabla w, \kappa \nabla \phi)_{L^2(\Omega)} = 0 \qquad \text{in } \Omega \times \mathcal{I}, \tag{102a}$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}) \quad \text{in } \Omega, \tag{102b}$$

where we use the standard notation for the function spaces with $H_g^1(\Omega) := \left\{ w \in H^1(\Omega) : w = g \text{ on } \partial\Omega \right\}$. We note that the this problem suits the abstract framework with function spaces $\mathcal{W} = H_g^1(\Omega), \mathcal{W}^* = H^{-1}(\Omega)$. The linear operator $\mathcal{L} : H_g^1(\Omega) \to H^{-1}(\Omega)$ is defined as

$${}_{H^{-1}(\Omega)}\langle \mathcal{L}\phi, w \rangle_{H_0^1(\Omega)} = (w, \partial_t \phi)_{L^2(\Omega)} - (\nabla w, \mathbf{a}\phi - \kappa \nabla \phi)_{L^2(\Omega)}. \tag{103}$$

Applying the methodology results in the following method:

find $\phi^h \in \mathcal{W}_g^h$ *such that for all* $w^h \in \mathcal{W}_0^h$*:*

$$\underbrace{(w^h, \partial_t \phi^h + \mathbf{a}\cdot\nabla\phi^h)_{L^2(\Omega)} + (\nabla w^h, \kappa\nabla\phi^h)_{L^2(\Omega)}}_{\text{Galerkin contribution}} + \underbrace{\sum_K ((\tau_{\text{CL}})_K(\mathbf{a}\cdot\nabla w^h + \kappa\Delta w^h), \mathscr{R}_{\text{CL}}\phi^h)_{L^2(\Omega_K)}}_{\text{VMS stabilization}}$$

$$+\left\{\begin{array}{ll} \underbrace{\sum_K (\nabla w^h, \nu_K \nabla\phi^h)_{L^2(\Omega_K)}}_{\substack{\text{Discontinuity capturing}\\ \text{in physical coordinates}}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla\phi^h\|_{\varepsilon,2} \\ \underbrace{\sum_K (\nabla_{\boldsymbol{\xi}} w^h, \nu_K \nabla_{\boldsymbol{\xi}}\phi^h)_{L^2(\Omega_K)}}_{\substack{\text{Discontinuity capturing}\\ \text{in reference coordinates}}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2} \end{array}\right\} = 0 \tag{104a}$$

where the variation entropy viscosity is:

$$\nu_{\text{VE}} = \left\{\begin{array}{ll} C\ h_Q^2 \left(\dfrac{\|\nabla\phi^h\|_{\varepsilon,2}}{|\!|\!|\nabla\phi^h|\!|\!|_{\varepsilon,\mathbf{G}}}\right)\dfrac{\left\{\mathcal{L}\left(\|\nabla\phi^h\|_{\varepsilon,2}\right)\right\}_+}{|\!|\!|\nabla\phi^h|\!|\!|_{\varepsilon,\mathbf{G}}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla\phi^h\|_{\varepsilon,2} \\ C\ h_Q^2 \dfrac{\left\{\mathcal{L}\left(\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}\right)\right\}_+}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}} & \textit{if} \quad \eta_\varepsilon^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}. \end{array}\right. \tag{104b}$$

We wish to emphasize that convection-diffusion and variation entropy operators coincide:

$$\mathscr{R}_{\text{CL}}\phi^h = \mathcal{L}\phi^h, \tag{105a}$$

$$\mathscr{R}_{\text{VE}}\eta^h = \mathcal{L}\eta^h. \tag{105b}$$

The element-wise stabilization parameter $(\tau_{\text{CL}})_K$ is defined as in [58].

3.11. Connection to the YZβ method

In order to establish the connection to the YZβ method [24] we present an alternative small-scale model. Instead of using the model (74), one can use an approximation. Using the definition (45) we may write:

$$\widehat{\{\eta'\}}_{-\text{VE}} = -\tau_{\text{VE}}\left\{\frac{\partial\eta^h}{\partial\nabla\phi^h}\cdot\nabla(\mathscr{R}_{\text{CL}}(\phi^h))\right\}_+ . \tag{106}$$

Again using (76) we now approximate (106) as a residual-based model via:

$$\begin{aligned} \widehat{\{\eta'\}}_{-\text{CL}} =& -\tau_{\text{VE}}\ h_Q^{-1}\left\|\mathbf{J}^{-1}\frac{\partial\eta^h}{\partial\nabla\phi^h}\right\|_2 \left|\mathscr{R}_{\text{CL}}\left(\phi^h\right)\right| \\ =& -\tau_{\text{VE}}\ h_Q^{-1}\left|\!\left|\!\left|\frac{\partial\eta^h}{\partial\nabla\phi^h}\right|\!\right|\!\right|_{\mathbf{G}} \left|\mathscr{R}_{\text{CL}}\left(\phi^h\right)\right|, \end{aligned} \tag{107}$$

Using the model (77) for $\mu\tau_{\mathrm{VE}}$, the corresponding variation entropy viscosity takes the form:

$$\nu_{\mathrm{CL}} = \mu\ \tau_{\mathrm{VE}}\ h_Q^{-1} \left\| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right\|_{\mathbf{G}} \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\eta^h} \tag{108}$$

$$= C\ h_Q \left\| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right\|_{\mathbf{G}}^{-1} \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\eta^h}\ , \tag{109}$$

where the subscript refers to the conservation law residual. In this case the variation entropy viscosity (108) scales with the residual of the conservation law but generally does not vanish when the variation entropy condition is satisfied.

Using the same large-scale variation entropies, i.e. $\eta^h = \|\nabla\phi^h\|_2$ and $\eta^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_2$, we get the expressions:

$$\eta^h = \|\nabla\phi^h\|_2 \quad \Rightarrow \quad \nu_{\mathrm{CL}} = C\ h_Q\ \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla\phi^h\|_{\mathbf{G}}}\ , \tag{110a}$$

$$\eta^h = \|\nabla_{\boldsymbol{\xi}}\phi^h\|_2 \quad \Rightarrow \quad \nu_{\mathrm{CL}} = C\ h_Q\ \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2}\ . \tag{110b}$$

Lemma 3.22. *On uniform Cartesian quadratic/cubic meshes we have*

$$\nu_{CL}\ (\|\nabla\phi^h\|_2) = C\ h_K \frac{|\mathscr{R}_{CL}\left(\phi^h\right)|}{\|\nabla\phi^h\|_2}, \tag{111a}$$

$$\nu_{CL}\ (\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2) = C\ h_Q \left(\frac{\partial x}{\partial \xi}\right)^{-1} \frac{|\mathscr{R}_{CL}\left(\phi^h\right)|}{\|\nabla\phi^h\|_2}. \tag{111b}$$

Proof. The proof is similar to that of Lemma 3.15 and uses (82b)-(82d). ☐

Corollary 3.23. *On uniform Cartesian quadratic/cubic meshes we have the identity:*

$$\nu_{CL}\ (\|\nabla\phi^h\|_2) = \left(\frac{\partial x}{\partial \xi}\right)^2 \nu_{CL}\ (\|\nabla_{\boldsymbol{\xi}}\phi^h\|_2). \tag{112}$$

The regularized versions of the variation entropy viscosities are:

$$\eta^h_\varepsilon = \|\nabla\phi^h\|_{\varepsilon,2} \quad \Rightarrow \quad \nu_{\mathrm{CL}} = C\ h_Q\ \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla\phi^h\|_{\varepsilon,\mathbf{G}}}\ , \tag{113a}$$

$$\eta^h_\varepsilon = \|\nabla_{\boldsymbol{\xi}}\phi^h\|^2_{\varepsilon_\xi,2} \quad \Rightarrow \quad \nu_{\mathrm{CL}} = C\ h_Q\ \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}}\ . \tag{113b}$$

Corollary 3.24. *On uniform Cartesian quadratic/cubic meshes we have the identity:*

$$\nu_{CL}\ (\|\nabla\phi^h\|_{\varepsilon,2}) = \left(\frac{\partial x}{\partial \xi}\right)^2 \nu_{CL}\ (\|\nabla_{\boldsymbol{\xi}}\phi^h\|_{\varepsilon_\xi,2}). \tag{114}$$

Theorem 3.25. *On uniform Cartesian quadratic/cubic meshes the choices $\eta = \|\nabla\phi\|_{\varepsilon,2}$ and $\eta = \|\nabla_{\boldsymbol{\xi}}\phi\|_{\varepsilon_\xi,2}$ coincide.*

Substitution yields weak formulation (98) where the variation entropy viscosity are now given by (113).

As variation entropy we take $\eta^h = \|\nabla\phi^h\|_2$ which yields:

$$\left(\nabla w^h, \mathbf{K}_K \nabla\phi^h\right)_{L^2(\Omega_K)} = \left(\nabla w^h, C\ h_Q \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla\phi^h\|_{\varepsilon,\mathbf{G}}}\nabla\phi^h\right)_{L^2(\Omega_K)}. \tag{115}$$

This is the (regularized version of the) discontinuity capturing term used by Akkerman et al. [44] for the level-set convection equation. On Cartesian uniform meshes it reduces to

$$\left(\nabla w^h, \mathbf{K}_K \nabla\phi^h\right)_{L^2(\Omega_K)} = \left(\nabla w^h, C\ h_K \frac{|\mathscr{R}_{\mathrm{CL}}\left(\phi^h\right)|}{\|\nabla\phi^h\|_{\varepsilon,2}}\nabla\phi^h\right)_{L^2(\Omega_K)}. \tag{116}$$

For convection-diffusion problems this coincides with the YZβ discontinuity capturing operator [24] with parameter $\beta = 1$. This term is used for non-uniform meshes as well.

Remark 3.26. Remark that YZβ discontinuity capturing and the beyond SUPG discontinuity capturing are nearly identical in a one dimensional pure convection case with stabilization parameter h/a.

Remark 3.27. The discontinuity capturing operator YZβ with parameter $\beta = 2$, in contrast to $\beta = 1$, does not fit in the presented framework. The fact that the choice $\beta = 1$ is preferred over $\beta = 2$, see [24], confirms the viability of the presented theory.

4. Numerical comparison

In this Section we evaluate the numerical methods on benchmark problems. All the computations are performed with tIGAr [63]. We employ C^1-continuous quadratic NURBS and use the generalized-α time-integrator with the parameter $\rho_\infty = 1.0$. Note that this is the only time-integrator within the generalized-α family linked to correct energy behavior, see e.g. [58]. The regularization parameter is taken as $\varepsilon^2 = 10^{-2}$.

We show the results of using

1. the well-known SUPG method.
2. the YZβ method with $\beta = 1$. The connection of this method with the developed framework is presented in Section 3.11.
3. the new method which is summarized in Section 3.9.

All the computations are performed on Cartesian meshes. Here the choices $\eta = \|\nabla\phi\|_2$ and $\eta = \|\nabla_{\boldsymbol{\xi}}\phi\|_2$ coincide (Theorem 3.20). Non-Cartesian computations may be subject of another work.

First we evaluate the convergence behavior of the new methods on a smooth pure advection problem. Then we evaluate the methods on two nonlinear benchmark problems: (i) the Buckley-Leverett equation with gravity and (ii) the KPP rotating wave problem. Both tests involve non-convex fluxes and are challenging since the corresponding solutions have a two-dimensional composite wave-structure. These problems have been employed in other works concerning discontinuity capturing mechanisms, see e.g. [24, 48, 64–66]. We refer the reader for a comparison of the results to those works.

4.1. Convergence on smooth solutions

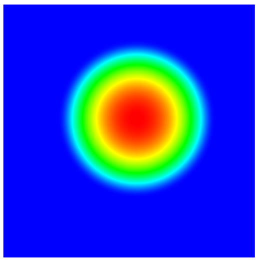
In this first numerical experiment we consider a smooth profile to test the convergence of the methods. The problem reads:

$$\partial_t\phi + \nabla\cdot\mathbf{f} = 0, \tag{117a}$$

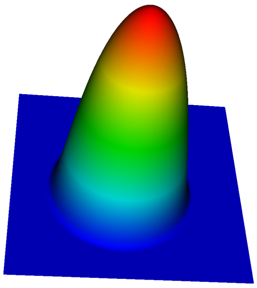
$$\phi(\mathbf{x},0) = \begin{cases} \exp\left(-\dfrac{1}{1-r^2}\right) & \text{if } r < 1.0, \\ 0.0 & \text{otherwise,} \end{cases} \tag{117b}$$

$$\mathbf{f}(\phi) = \mathbf{a}\phi. \tag{117c}$$

with radius $r = \sqrt{x^2 + y^2}$.



(a) 2D topview



(b) 3D sideview

Figure 2: Smooth solution problem with quadratic NURBS. The final solution at $t = 1.0$.

The convection velocity field is constant with value $\mathbf{a} = (0.1, 0.15)$. The time-step size is chosen as $\Delta t = 4h_K$ and we take $C = 0.5$. Figure 3 shows second-order/third-order convergence in the L^2-norm for each of the three methods which for finer meshes yields second-order convergence due to the choice of the time-integrator.

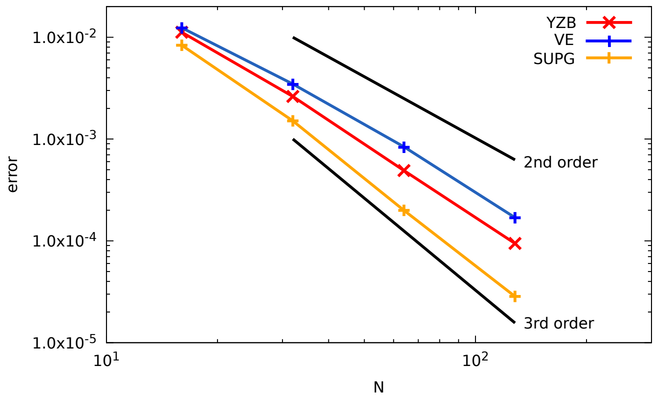


Figure 3: L^2 convergence of the smooth solution problem with quadratic NURBS.

4.2. Buckley-Leverett with gravity

The gravitational Buckley-Leverett problem with a Riemann initial configuration reads:

find $\phi = \phi(\mathbf{x}, t) : \Omega \times \mathcal{I} \to \mathbb{R}$ *such that:*

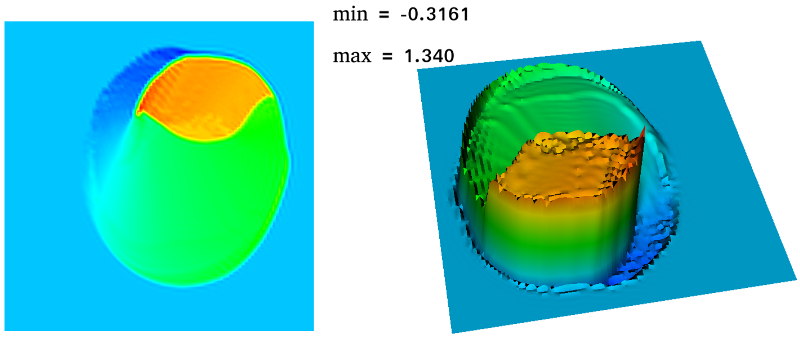
$$\partial_t \phi + \nabla \cdot \mathbf{f} = 0, \tag{118a}$$

$$\phi(\mathbf{x}, 0) = \begin{cases} 1.0 & \text{if } x^2 + y^2 \leq 0.5, \\ 0.0 & \text{otherwise,} \end{cases} \tag{118b}$$

$$\mathbf{f}(\phi) = \left(\frac{\phi^2}{\phi^2 + (1-\phi)^2}, \frac{\phi^2(1 - 5(1-\phi)^2)}{\phi^2 + (1-\phi)^2}) \right). \tag{118c}$$

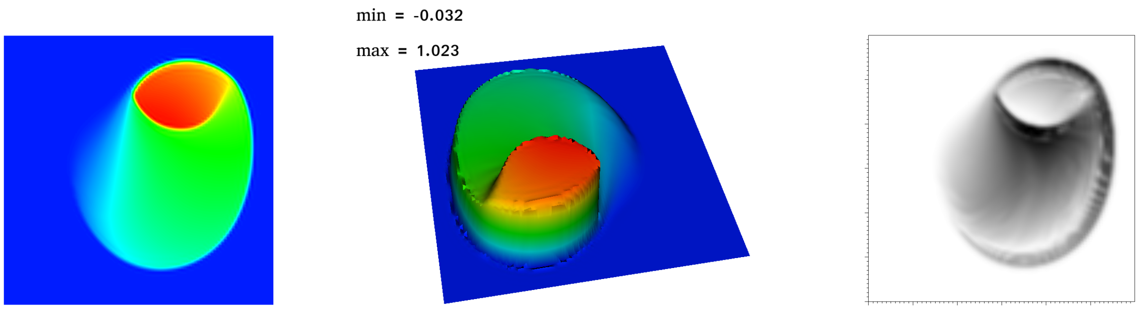
The Buckley-Leverett problem emerges from a two-phase immiscible incompressible fluid problem. It represents a saturation equation in which gravitational effects are incorporated. This results in different fluxes in both spatial directions. The problem has also been considered in [48, 66, 67]. The solution is advanced in time until $t = 0.5$.

All computations are performed on a 100x100 mesh with time-step size $\Delta t = 0.01$. We show in Figures 4-6 the solution profiles at final time $t = 0.5$. The gray scale of the viscosity magnitude is per Figure chosen such that the location of the diffusion becomes most apparent. The results of the SUPG method contain excessive oscillations. The discontinuity capturing viscosity based on the variation entropy condition focuses on the sharp layer, whereas basing it on the residual of the conservation law spreads it out.



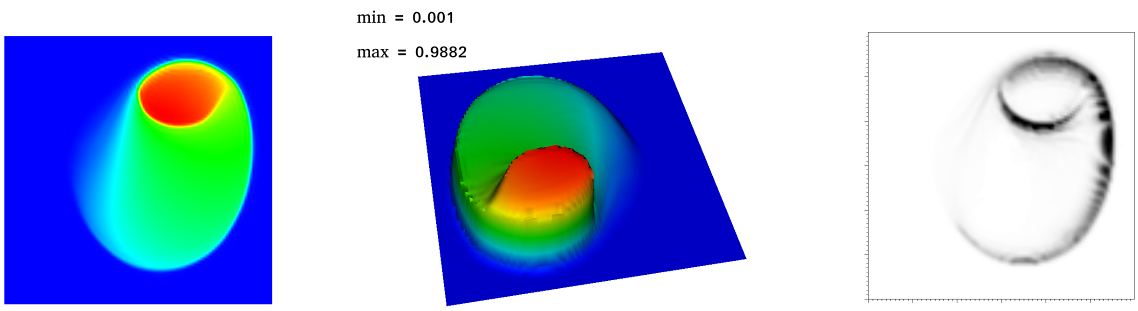
(a) 2D topview (b) 3D sideview

Figure 4: Buckley-Leverett problem, the solution at final time $t = 0.5$ using the SUPG method.



(a) 2D topview (b) 3D sideview (c) viscosity magnitude

Figure 5: Buckley-Leverett problem, the solution at final time $t = 0.5$ using the YZβ method with constant $C = 0.25$.



(a) 2D topview (b) 3D sideview (c) viscosity magnitude

Figure 6: Buckley-Leverett problem, the solution at final time $t = 0.5$ using the VE method with constant $C = 0.25$.

4.3. KPP rotating wave

The KPP rotating wave problem is:

find $\phi = \phi(\mathbf{x}, t) : \Omega \times \mathcal{I} \to \mathbb{R}$ *such that:*

$$\partial_t \phi + \nabla \cdot \mathbf{f} = 0, \tag{119a}$$

$$\phi(\mathbf{x}, 0) = \begin{cases} 3.5\pi & \text{if } x^2 + y^2 \leq 1, \\ 0.25\pi & \text{otherwise,} \end{cases} \tag{119b}$$

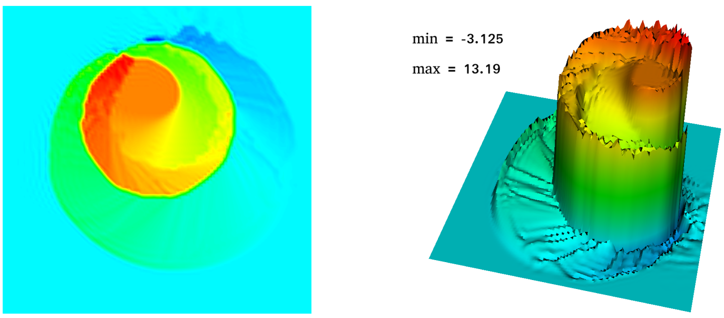
$$\mathbf{f}(\phi) = (\sin \phi, \cos \phi) \, . \tag{119c}$$

The test case was proposed in [65] and is named after the authors Kurganov, Petrova, and Popov. Several reconstruction schemes, e.g. central-upwind schemes as WENO5, Minmod 2 and SuperBee, are not successful for this test.

All computations are performed on a 100x100 mesh with time-step size $\Delta t = 0.01$. Figures 7-9 show the solution profiles of the various methods at final time $t = 1$.

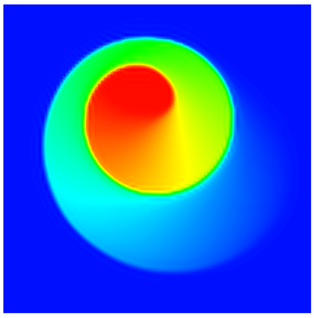
The results of the SUPG method display sharp layers with excessive oscillations. The solution quality improves greatly when using any of the other methods. Again, the discontinuity capturing viscosity is more localized near the sharp layers when it is based on the variation entropy condition (displayed in Figure 9) than on the residual of the conservation law (see Figure 8). We see at some locations a viscosity value that is higher than required. In Figure 10 we show the results of using a maximum for the viscosity via equation (100) with $C_{\max} = 1.0$. The gray scale of the viscosity magnitude of Figures 9 and 10 is the same to highlight the effect of using a maximum viscosity. The overly diffusive regions are now removed and the resulting profile has minimal smearing and the spurious oscillations are virtually absent.

Remark 4.1. In this testcase it is apparent that the viscosity of the new method is active in regions where variation entropy is created. Gibbs oscillations appear right next to the discontinuity and this is where the viscosity acts. Note that the viscosity is absent at the location of the shockwave itself. This is in contrast to the entropy viscosity method [48] in which the viscosity focuses on the shockwave itself rather than on the oscillations next to it.

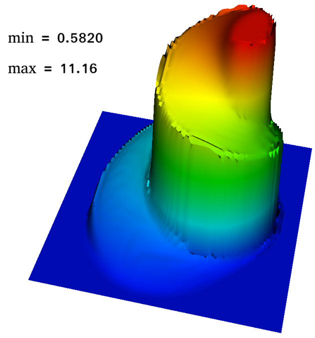


(a) 2D topview (b) 3D sideview

Figure 7: KPP rotating wave problem, the solution at final time $t = 1.0$ using the SUPG method.



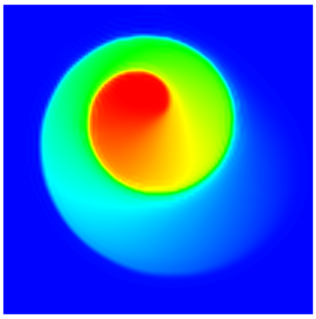
(a) 2D topview



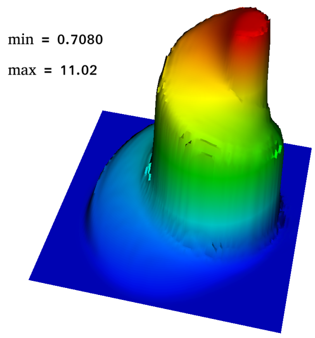
(b) 3D sideview

(c) viscosity magnitude

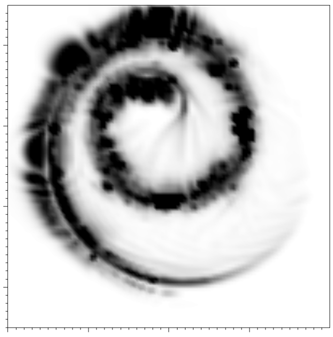
Figure 8: KPP rotating wave problem, the solution at final time $t = 1.0$ using the YZβ method with constant $C = 0.25$.



(a) 2D topview

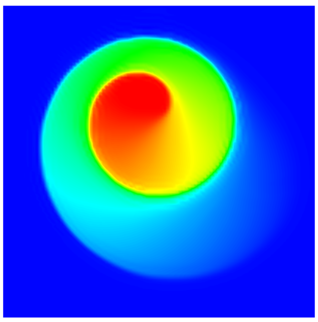


(b) 3D sideview

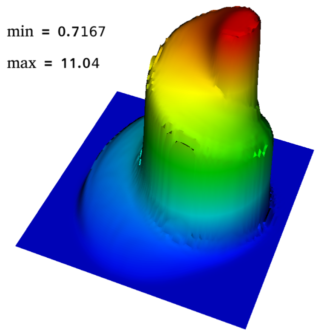


(c) viscosity magnitude

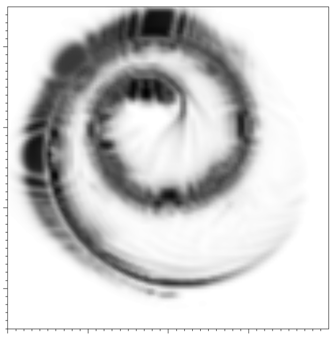
Figure 9: KPP rotating wave problem, the solution at final time $t = 1.0$ using the VE method with constant $C = 0.25$.



(a) 2D topview



(b) 3D sideview



(c) viscosity magnitude

Figure 10: KPP rotating wave problem, the solution at final time $t = 1.0$ using the VE method with constant $C = 0.25$ and using the maximum viscosity (100).

5. Conclusions

In this paper we have presented a general framework for discontinuity capturing mechanisms. The framework does not employ *ad hoc* devices which is, to the best knowledge of the authors, in contrast to previous discontinuity capturing methods. The developed theory contains two key ingredients, namely variation entropy theory and variational multiscale analysis. Variation entropy provides us the location of the viscosity and VMS models this viscosity via the missing scales. Merging the variation entropy concept into the variational multiscale method naturally equips the variational multiscale method with a discontinuity capturing term.

The discontinuity capturing viscosity is based on the variation entropy condition. In smooth regions the variation entropy relation is governed with an equality, and this is where the discontinuity capturing term vanishes. Near sharp layers, however, the variation entropy relation becomes an inequality. Here the discontinuity capturing term switches on; dissipation based on the variation entropy production is added to the formulation.

Many spurious oscillation diminishing methods are isotropic of nature or add diffusion in the crosswind direction. The discontinuity capturing viscosity acts in the direction identified by the change of the variation entropy. We believe that this is a natural direction, since this is where sharp layers are expected. In particular cases the viscosity reduces to an isotropic one.

The steps of the framework to arrive at a discontinuity capturing term can be summarized as follows:

1. Regularize the conservation law.
2. Perform a multiscale split and subsequently take the limit of regularization parameter to zero.
3. Select a projector based on the variation entropy condition.
4. Select a small-scale variation entropy model.
5. Compute the variation entropy viscosity.
6. Select a large-scale variation entropy.

We have tested the new discontinuity capturing method on nonlinear benchmark problems. The computations are performed with quadratic NURBS. The numerical results are virtually oscillation-free and have minimal smearing. Compared to the well-known YZβ method [24], the diffusion of the new discontinuity method is more localized *near* sharp layers. These are the locations where variation entropy can be created. We emphasize that the diffusion should not be added at the shock but right next to it.

This paper sheds light on the different concepts of entropy solutions, the total variation diminishing property and their relation to discontinuity capturing mechanisms. In particular, it establishes a connection between total variation/variation entropy and discontinuity capturing.

The current framework provides some insight into discontinuity capturing techniques, however we certainly do not claim that it is sufficient in this context. There are several openings.

- The first concerns the choice of the variation entropy. Numerical results indicate that taking the 2-norm of the gradient leads to good behavior. Improvement might be achieved with another choice of the variation entropy.
- Another point that deserves interest is the small-scale variation entropy model. We have taken the simplest options and perhaps at this point progress can be made.
- Furthermore, a numerical investigation of the performance of the new method on curved/non-Cartesian meshes could be investigated.

Summarizing, this paper proposes a novel paradigm for the construction of discontinuity capturing operators. We think that the framework has a more fundamental mathematical foundations than previously proposed methods. The reason is that it naturally emerges from the conservation law and does not contain ad hoc devices. This, together with the good numerical results illustrate the viability of the framework. The basic questions of discontinuity capturing operators, i.e. (i) where to add diffusion?, and (ii) how much diffusion should be added? are answered. The results of this paper indicate that diffusion should be added there where variation entropy is being produced with an amount that scales with the variation entropy production.

We close this paper with the following note. The variational multiscale method has proven to be a powerful tool for the simulation of turbulent flows, as displayed in the seminal work [37]. In the current paper we have demonstrated that, in addition to this,

the variational multiscale method is suitable to deal with sharp layers/discontinuities.

The reason for this is simple: both turbulence and shock wave problems contain features that do not 'fit' on a coarse mesh; the variational multiscale framework incorporates these features into the numerical method.

Appendix A. An alternative optimality projector

Here we present an alternative projector that directly penalizes violation of the variation entropy condition. Consider the minimization problem:

find $\phi^h \in \mathcal{W}^h$ such that:

$$\mathscr{L}(\phi - \phi^h) = \inf_{\theta^h \in \mathcal{K}^h} \mathscr{L}(\phi - \theta^h), \tag{A.1}$$

where the constraint set reads:

$$\mathcal{K}^h := \left\{ \phi^h \in \mathcal{W}^h : \; (v^h, \mathscr{R}_{\mathrm{VE}} \eta^h)_{L^2(\Omega)} \leq 0 \quad \text{for all } v^h \in \mathcal{V}^h \right\}. \tag{A.2}$$

We proceed by opening the solution space with a penalty approach. We define the projector by

$$\mathscr{P}^h \phi = \underset{\phi^h \in \mathcal{W}^h}{\arg\min} \left\{ \frac{1}{2} \left\| \phi - \phi^h \right\|_{\mathcal{W}}^2 + \frac{1}{2} \left\| \sqrt{\mu} \tau_{\mathrm{VE}} \{ \mathscr{R}_{\mathrm{VE}} \eta^h \}_+ \right\|_{L^2(\Omega)}^2 \right\}, \tag{A.3}$$

where μ and τ_{VE} play the same role as before. Just like for the projector of Section 3.5, when the variation entropy condition is not harmed the first-order optimality conditions reduce to an $H^1(\Omega)$ orthogonality. This optimality projector $\mathscr{P}^h$ implies:

find $\phi^h \in \mathcal{W}^h$ such that, for all $w^h \in \mathcal{W}^h$

$$\left(\phi', w^h \right)_{\mathcal{W}} = \left(\mu \tau_{\mathrm{VE}}^2 \{ \mathscr{R}_{\mathrm{VE}} \eta^h \}_+, \mathrm{d} \mathscr{R}_{\mathrm{VE}} \eta^h (\nabla \phi^h)(\nabla w^h) \right)_{L^2(\Omega)}. \tag{A.4}$$

Employing the definition of $\mathscr{R}_{\mathrm{VE}}$ and the chain rule we arrive at:

$$\begin{aligned} \left(\phi', w^h \right)_{\mathcal{W}} = & \left(\mu \tau_{\mathrm{VE}}^2 \{ \mathscr{R}_{\mathrm{VE}} \eta^h \}_+ \frac{\partial \eta^h}{\partial \nabla \phi^h}, \mathrm{d} \left(\nabla \mathscr{R}_{\mathrm{CL}} \right) (\phi^h)(w^h) \right)_{L^2(\Omega)} \\ & + \left(\mu \tau_{\mathrm{VE}}^2 \{ \mathscr{R}_{\mathrm{VE}} \eta^h \}_+, \mathbf{H}_{\nabla \phi^h} \eta^h \nabla w^h, \nabla \mathscr{R}_{\mathrm{CL}} \phi^h \right)_{L^2(\Omega)}. \end{aligned} \tag{A.5}$$

Using the homogeneity property and interchanging differential operators we may write:

$$\left(\phi', w^h \right)_{\mathcal{W}} = \left(\mathbf{K} \nabla \phi^h, \tau_{\mathrm{VE}} \nabla \left(\mathrm{d} \mathscr{R}_{\mathrm{CL}} (\phi^h)(w^h) \right) \right)_{L^2(\Omega)} + \left(\bar{\mathbf{K}} \nabla w^h, \tau_{\mathrm{VE}} \nabla \mathscr{R}_{\mathrm{CL}} \phi^h \right)_{L^2(\Omega)}. \tag{A.6}$$

where τ_{VE} denotes the time-scale linked to the variation entropy and where the matrices are given by:

$$\mathbf{K} = \nu_{\mathrm{VE}} \frac{\partial \eta^h}{\partial \nabla \phi^h} \otimes \frac{\partial \eta^h}{\partial \nabla \phi^h}, \tag{A.7a}$$

$$\bar{\mathbf{K}} = \nu_{\mathrm{VE}} \eta^h \mathbf{H}_{\nabla\phi} \eta^h, \tag{A.7b}$$

$$\nu_{\mathrm{VE}} = \mu \tau_{\mathrm{VE}} \frac{\{\mathscr{R}_{\mathrm{VE}} \eta^h\}_+}{\eta^h}. \tag{A.7c}$$

We arrive at the same expression for ν_{VE}, we may employ the model (77). At this point it is unclear how to arrive at a numerical method from the small-scale model. There are several options however these include unwanted approximations and/or require neglecting some terms. We do not proceed with this projector however we present some discussion on the diffusion matrices below.

Proposition Appendix A.1. *The matrices* $\mathbf{K}$ *and* $\bar{\mathbf{K}}$ *are symmetric positive semi-definite.*

Proof. Symmetry is trivial and the positive semi-definiteness of is a direct consequence of ν_{VE} being positive and the convexity of η^h (for $\bar{\mathbf{K}}$). □

Note that both $\mathbf{K}$ and $\bar{\mathbf{K}}$ have the unit of a viscosity and both are based on the variation entropy residual. The matrix $\mathbf{K}$ is the same as found before and acts in the direction is represented by $\partial\eta/\partial\nabla\phi^h$. Below we analyze the matrix $\bar{\mathbf{K}}$.

Let $\mathbf{u}_{||}$ denote the projection of $\mathbf{u}$ onto $\partial\eta/\partial\nabla\phi^h$:

$$\mathbf{u}_{||} := \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \otimes \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \mathbf{u} \tag{A.8}$$

where the hat-symbol indicates scaling to unit size: $\hat{\mathbf{v}} = \mathbf{v}/\|\mathbf{v}\|_2$. Note that we have the identity

$$\mathbf{u}_{||} \cdot \frac{\partial \eta^h}{\partial \nabla \phi^h} = \mathbf{u} \cdot \frac{\partial \eta^h}{\partial \nabla \phi^h}, \tag{A.9}$$

and that the vector

$$\mathbf{u}_{\perp} := \mathbf{u} - \mathbf{u}_{||} = \left(\mathbf{I} - \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \otimes \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \right) \mathbf{u} \tag{A.10}$$

is perpendicular to $\mathbf{u}$. Whereas the matrix $\mathbf{K}$ provides control over gradient in the direction $\partial\eta/\partial\nabla\phi^h$ (represented by $\mathbf{u}_{||}$), the matrix $\bar{\mathbf{K}}$ can provide control of gradients in the direction orthogonal to that (represented by $\mathbf{u}_{\perp}$). In this case $\bar{\mathbf{K}}\mathbf{u}$ should be proportional to $\mathbf{u}_{\perp}$. This is only the case if $\eta = \|\nabla\phi^h\|_2$, as stated in the next proposition.

Proposition Appendix A.2. *The matrix* $\bar{\mathbf{K}}$ *acts in the direction orthogonal to* $\partial\eta/\partial\nabla\phi^h$ *if and only if* $\eta = \|\nabla\phi^h\|_2$ *(up to multiplication with a constant).*

Proof. Up to scaling by a constant, we need to find η^h such that:

$$\bar{\mathbf{K}}\mathbf{u} = \nu_{\mathrm{VE}} \mathbf{u}_{\perp} \tag{A.11}$$

for all vectors $\mathbf{u}$. Substitution of (A.7b) and (A.10) gives:

$$\nu_{\mathrm{VE}} \eta^h \mathbf{H}_{\nabla\phi^h} \eta \mathbf{u} = \nu_{\mathrm{VE}} \left(\mathbf{I} - \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \otimes \frac{\hat{\partial \eta^h}}{\partial \nabla \phi^h} \right) \mathbf{u}. \tag{A.12}$$

Taking $\mathbf{u} = \nabla \phi^h$ provides

$$\eta^h \mathbf{H}_{\nabla \phi^h} \eta \nabla \phi^h = \nabla \phi^h - \eta^h \frac{\partial \hat{\eta}^h}{\partial \nabla \phi^h} \left\| \frac{\partial \eta}{\partial \nabla \phi^h} \right\|_2^{-1}. \tag{A.13}$$

Next, we use the homogeneity property (12) to find:

$$\nabla \phi^h - \eta^h \frac{\partial \hat{\eta}^h}{\partial \nabla \phi^h} \left\| \frac{\partial \eta}{\partial \nabla \phi^h} \right\|_2^{-1} = 0. \tag{A.14}$$

Rearranging gives

$$\left\| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right\|_2 \nabla \phi^h = \frac{\partial \hat{\eta}^h}{\partial \nabla \phi^h} \eta^h. \tag{A.15}$$

Taking the norm leads to:

$$\left\| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right\|_2 \left\| \nabla \phi^h \right\|_2 = \eta^h. \tag{A.16}$$

By again using homogeneity we arrive at

$$\left\| \frac{\partial \eta^h}{\partial \nabla \phi^h} \right\|_2 \left\| \nabla \phi^h \right\|_2 = \frac{\partial \eta^h}{\partial \nabla \phi^h} \cdot \nabla \phi^h. \tag{A.17}$$

This means that the vectors $\partial \eta / \partial \nabla \phi^h$ and $\nabla \phi^h$ point in the same direction. We conclude $\eta = \| \nabla \phi^h \|_2$, up to multiplication with a constant. □

Acknowledgment

The authors want to thank David Kamensky for fruitful discussions and providing assistance with the open source library tIGAr. YB was partially supported by the NSF Award No. 1854436.

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