MESH MOVEMENT GOVERNED BY ENTROPY PRODUCTION

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ABSTRACT

The aim of this paper is to study the feasibility of using (irreversible) entropy production as driving force for a moving mesh. Such a method should be able to capture or track physical phenomena such as viscous and thermal boundary layers, shock waves and regions with chemical reactions.
A brief outline is given for the FEM-ALE approach, which forms the basis of the moving mesh method. Mesh velocity is a degree of freedom when the Arbitrary-Lagrangian-Eulerian (ALE) formulation for governing PDEs is used. A Finite Element Method (FEM, viz. Galerkin's method) is applied as discretization of the spatial domain.
Two methods will be suggested for determination of mesh motion: mesh displacement method and mesh velocity method. Both methods have an analogy with respectively solid mechanics and fluid mechanics. The general PDE for mesh motion is based on the equation of motion used in continuum mechanics. Body force for mesh motion is determined by temperature and the gradient of entropy production. This implementation introduces a coupling between mesh motion and the governing physics.
The suggested method is implemented in the commercial software package FEMLAB® (release 3.0a). A heat conduction problem in a 1-dimensional geometry is selected as physical problem. Numerical solutions for both mesh methods are shown. For the mesh velocity method the geometry is also extended with a prescribed moving boundary. Finally, there are some remarks about stabilization methods for convection-dominated problems.

Keywords: arbitrary Lagrangian-Eulerian formulation, moving mesh, entropy production

1. INTRODUCTION

A moving mesh method has a fixed mesh topology (i.e. number of vertices and connectivity), while only the mesh vertices move with time. Such a mesh is only useful in combination with non-stationary physical problems. In this paper, an adaptive mesh is considered to be a modification of the mesh topology and is often used for stationary physical problems. Such a method could be used to create an initial mesh for a moving mesh problem. Since the main topic of this paper is determination of mesh motion, the actual physical problem is of less importance. The focus will be on physical problems consisting of arbitrary transport phenomena.

The physical problem is, in general, governed by a set of conservative laws (e.g. mass, linear momentum and energy). The required constitutive relations are, among other criteria, based on the entropy principle (see references on thermoelasticity, e.g. [1, 2, 3]). This paper will study the feasibility of using entropy production as driving force for a moving mesh method. The objective is to obtain a governing PDE for a moving mesh that is capable of *both* refining the mesh at interesting regions and handling arbitrary moving boundaries. An advantage of using only PDEs for determining mesh motion is the lack of iteration loops required for finding an optimal mesh (such as with error estimation methods). One of the criteria that should be checked is whether the mesh stops moving if an equilibrium state is obtained. The arbitrary Lagrangian-Eulerian (ALE) formulation includes a moving mesh into the system of PDEs, so there are no projection errors due to remeshing.

The paper starts with a brief outline of the FEM-ALE approach, which introduces mesh velocity (and therefore mesh motion) as degree of freedom. Mesh motion is determined by solving an additional set of PDE(s) similtaneous with the set of physical PDE(s). The next section will introduce various PDEs for mesh motion based on physical analogies and concepts. Some of these PDEs are implemented in the commercial software package FEMLAB® in combination with a non-stationary convection-diffusion problem. Numerical results are shown for both fixed boundaries and a prescribed moving boundary. This section consists also of a brief introduction to combining the suggested approach with stabilization methods.

2. FEM-ALE APPROACH

The FEM-ALE approach is a method for numerically approximating master balance laws for an arbitrary set of quantities $\boldsymbol{\phi}$. These quantities can change due to any combination of surface sources $\boldsymbol{j}_{\boldsymbol{\phi}}$ and volumetric sources $\boldsymbol{\sigma}_{\boldsymbol{\phi}}$, viz.

$$\frac{\partial}{\partial t}\int_{\boldsymbol{\chi}|_t(\Omega_{\boldsymbol{z}})} \boldsymbol{\phi}\,\mathrm{d}V\bigg|_{\boldsymbol{z}} = -\int_{\boldsymbol{\chi}|_t(\partial\Omega_{\boldsymbol{z}})} \boldsymbol{n}\cdot\boldsymbol{j}_{\boldsymbol{\phi}}\,\mathrm{d}S + \int_{\boldsymbol{\chi}|_t(\Omega_{\boldsymbol{z}})} \boldsymbol{\sigma}_{\boldsymbol{\phi}}\,\mathrm{d}V. \quad (1)$$

Symbol $\boldsymbol{n}$ denotes the outwards pointing normal vector of surface element $\mathrm{d}S$. Integrands in above equation depend on *moving* spatial coordinate $\boldsymbol{y}$ and time t. The integration limits are determined by a moving material configuration $\Omega_{\boldsymbol{z}}$, where the corresponding spatial coordinates are specified by *physical* motion (see also figure 1)

$$\boldsymbol{y} = \boldsymbol{\chi}(\boldsymbol{z}, t) = \boldsymbol{\chi}|_t\,(\boldsymbol{z}) \quad (2)$$

A bar with a subscript is used to denote that the subscript is fixed.

The arbitrary Lagrangian-Eulerian formulation ([4, 5, 6]) is used to obtain an equivalent localized system of equations (PDEs) of the master balance laws for calculation domains with arbitrary moving boundaries. The system of PDEs is spatially discretized by a finite element method (i.e. Galerkins method, [7, 8]) to obtain a system of ODEs. These equations are integrated numerically with respect to time (see also [9]).

2.1 Arbitrary Lagrangian-Eulerian formulation

The governing concept of the ALE formulation is to let *both* a spatial configuration $\Omega_{\boldsymbol{y}}$ and a material configu-

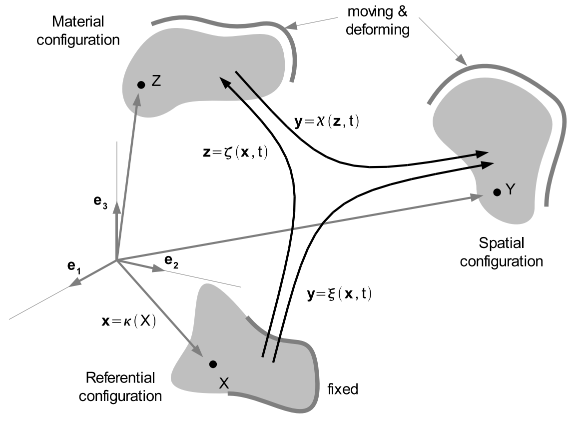

Figure 1: Relation between (moving) configurations and motions.

ration $\Omega_{\boldsymbol{z}}$ move and deform independently over a *fixed* referential configuration $\Omega_{\boldsymbol{x}}$. This introduces the spatial motion $\boldsymbol{\xi}$ as additional degree of freedom, which is independent of the physical motion $\boldsymbol{\chi}$. Figure 1 shows the relation between the various configurations and motions. It is emphasized that both spatial and physical motion map onto the spatial configuration, but they have different spatial coordinates.

Define physical velocity $\boldsymbol{v}$ as material derivative (i.e. time derivative at constant material coordinate $\boldsymbol{z}$) of physical motion, or

$$\frac{\partial}{\partial t}\boldsymbol{\chi}(\boldsymbol{z}, t)\bigg|_{\boldsymbol{z}} = \boldsymbol{v}(\boldsymbol{\chi}(\boldsymbol{z}, t), t) = \boldsymbol{v}(\boldsymbol{y}, t). \quad (3)$$

Similar, spatial velocity $\breve{\boldsymbol{v}}$ is defined as time derivative at constant referential coordinate $\boldsymbol{x}$

$$\frac{\partial}{\partial t}\boldsymbol{\xi}(\boldsymbol{x}, t)\bigg|_{\boldsymbol{x}} = \breve{\boldsymbol{v}}(\boldsymbol{\xi}(\boldsymbol{x}, t), t) = \breve{\boldsymbol{v}}(\boldsymbol{y}, t). \quad (4)$$

A generalised form of Reynolds transport theorem for an arbitrary region $\Omega(t)$ can then be derived for the ALE formulation (see [9])

$$\frac{\partial}{\partial t}\int_{\Omega(t)} \boldsymbol{\phi}\,\mathrm{d}V = \int_{\Omega(t)} \frac{\partial\boldsymbol{\phi}}{\partial t} + \boldsymbol{\phi}(\nabla\cdot\breve{\boldsymbol{v}}) + \nabla\cdot[(\boldsymbol{v}-\breve{\boldsymbol{v}})\otimes\boldsymbol{\phi}]\mathrm{d}V. \quad (5)$$

Notice that the single term of the left-hand side in equation (1) is transformed into three terms. Material derivative of quantity $\boldsymbol{\phi}$ is converted in a combination of: local time derivative, volume dilatation (shown by divergence of spatial velocity) and convective flow.

Above equation changes the sequence of time differentiation and volume integration. The master balance law (1) can be written as a single integral equal to zero by using above kinematical relation. Since the integration is over an arbitrary volume, the integrand has to be equal to zero. This yields an equivelent set of PDEs of equation (1), i.e.

$$\frac{\partial \boldsymbol{\phi}}{\partial t} + \boldsymbol{\phi}(\nabla \cdot \breve{\boldsymbol{v}}) + \nabla \cdot [(\boldsymbol{v} - \breve{\boldsymbol{v}}) \otimes \boldsymbol{\phi}] = -\nabla \cdot \boldsymbol{j}_{\boldsymbol{\phi}} + \boldsymbol{\sigma}_{\boldsymbol{\phi}}. \quad (6)$$

It is convenient to introduce the *relative* derivative as new differential operator by

$$\mathcal{D}\boldsymbol{\phi} = \frac{\partial \boldsymbol{\phi}}{\partial t} + (\boldsymbol{v} - \breve{\boldsymbol{v}}) \cdot \nabla \otimes \boldsymbol{\phi}, \quad (7)$$

such that equation (6) can be written as

$$\mathcal{D}\boldsymbol{\phi} = -\nabla \cdot \boldsymbol{j}_{\boldsymbol{\phi}} + \boldsymbol{\sigma}_{\boldsymbol{\phi}} - \boldsymbol{\phi}(\nabla \cdot \boldsymbol{v}). \quad (8)$$

The term denoting volume dilatation in equation (6) is in above equation considered to be a source term, because a changing geometry results in a change of density $\boldsymbol{\phi}$. Note that it consists of divergence of *physical* velocity instead of divergence of *spatial* velocity.

2.2 Finite element method

The ALE-formulation can be applied to domains with arbitrary moving and deforming calculation domains (i.e. geometries). The FEM-ALE approach combines the ALE-formulation with a finite element method to obtain a moving mesh method.

Equation (8) yields the problem statement in strong form and will be written in the corresponding weak form. Introduce a class of trial solutions $\mathcal{S}$ and a class of weighting functions $\mathcal{V}$. The weak form of equation (8) is obtained by multiplying with an arbitrary weight function $\boldsymbol{w} \in \mathcal{V}$ and integrating over an arbitrary spatial volume. The weak form yields then, $\forall \boldsymbol{w} \in \mathcal{V}$ find $\boldsymbol{\phi} \in \mathcal{S}$ such that

$$\begin{aligned} &\int_{\boldsymbol{\xi}|_t(\Omega_{\boldsymbol{x}})} \boldsymbol{w} \cdot \mathcal{D}\boldsymbol{\phi} \, \mathrm{d}V + \\ &\quad \int_{\boldsymbol{\xi}|_t(\Omega_{\boldsymbol{x}})} (\nabla \otimes \boldsymbol{w}) \cdot \boldsymbol{j}_{\boldsymbol{\phi}} \, \mathrm{d}V = \\ &\quad \int_{\boldsymbol{\xi}|_t(\Omega_{\boldsymbol{x}})} \boldsymbol{w} \cdot [\boldsymbol{\sigma}_{\boldsymbol{\phi}} - \boldsymbol{\phi}(\nabla \cdot \boldsymbol{v})] \, \mathrm{d}V + \\ &\quad \int_{\boldsymbol{\xi}|_t(\partial\Omega_{\boldsymbol{x}})} \boldsymbol{w} \cdot \boldsymbol{h}_{\boldsymbol{\phi}} \, \mathrm{d}S. \end{aligned} \quad (9)$$

Symbol $\boldsymbol{h}_{\boldsymbol{\phi}}$ denotes a Neumann boundary condition on some part of the boundary ($\partial\Omega_{\boldsymbol{y},N} \subset \partial\Omega_{\boldsymbol{y}}$) and originates from integration by parts.

The semi-discrete Galerkin formulation [7, 10] is applied to the weak form to get a spatial discretized formulation. This yields a system of first order ODEs with respect to time that can be (numerically) integrated. Equations of the form given by equation (9) can be implemented directly in the commercial software package FEMLAB® for domains with *fixed* boundaries. An algorithm for the moving boundaries is implemented in MATLAB®, using the MATLAB®-interface of FEMLAB® ([9, 11]).

Both the master balance laws and the weak form are with respect to (moving) spatial coordinates. Integration limits of the weak form are determined by spatial motion, instead of physical motion, so moving and deforming geometries can be described. Partition of weak form transforms *spatial* motion and velocity into *mesh* motion and velocity. Aim of this work is to obtain a generalized relation (PDEs) for determination of mesh motion (i.e. $\boldsymbol{\xi}$), where the basic idea is to govern mesh movement by physics (viz. entropy production).

3. PDE FOR MESH MOTION

Mesh motion is a degree of freedom in the FEM-ALE approach. In this paper a model for mesh motion is suggested, that is based on similarities with physics:

- Mesh motion is governed by a law of dynamics, analogous to continuum mechanics (i.e. Euler's first law, Cauchy's first law).
- Linear momentum of mesh elements is defined similar to linear momentum of a material volume.
- Gradient of entropy production acts as body force. The underlying idea is that a region with a large gradient of entropy production should have a refined mesh, while a region with a low gradient of entropy production could do with a course mesh. Entropy production is used, since it is a generic quantity arising for all non-ideal physical phenomena. Though the actual value of entropy production can not be predicted, it's sign is always positive. The gradient of entropy production can be either positive or negative and can thus result in both refining and coarsening of the mesh.
- Traction acts as a resisting force (contact force) to motion or deformation of mesh elements. The mode of resistance depends on the model for traction (or stress tensor), which could be based on similarities with either solid mechanics or fluid mechanics.

This model will be more elaborately introduced in the proceeding section, which is followed by both a solid mechanics approach and a fluid mechanics approach.

3.1 Basic idea

Define linear momentum $\boldsymbol{p}$ of an arbitrary mesh element $\Omega^e_{\boldsymbol{x}}$ as product of some multiplier ψ and mesh velocity $\dot{\boldsymbol{\xi}}$, viz.

$$\boldsymbol{p}(t) = \int_{\Omega_{\boldsymbol{x}}^e} \psi(\boldsymbol{x})\dot{\boldsymbol{\xi}}(\boldsymbol{x},t)\,\mathrm{d}V. \qquad (10)$$

Evaluate time derivative of linear momentum as referential derivative of the RHS integral and use time independence of multiplier ψ and configuration $\Omega_{\boldsymbol{x}}^e$ to get

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \int_{\Omega_{\boldsymbol{x}}^e} \psi\, \frac{\partial}{\partial t}\dot{\boldsymbol{\xi}}\bigg|_{\boldsymbol{x}} \mathrm{d}V. \qquad (11)$$

Since the physical problem is specified by spatial coordinates, it is convenient to transform above equation to these coordinates using the change of variables theorem. Define multiplier ψ as product of mass density and the Jacobian determinant of spatial motion

$$\psi\left(\boldsymbol{\xi}^{-1}(\boldsymbol{y},t)\right) = \rho(\boldsymbol{y},t)\det(\mathsf{J}_{\boldsymbol{\xi}})(\boldsymbol{y},t). \qquad (12)$$

Time derivative of linear momentum of mesh elements can then be written as

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \int_{\boldsymbol{\xi}|_t(\Omega_{\boldsymbol{x}}^e)} \rho\, \frac{\partial \breve{\boldsymbol{v}}}{\partial t}\bigg|_{\boldsymbol{x}} \mathrm{d}V, \qquad (13)$$

where the integrand is with respect to spatial coordinates and time. This relation can be interpreted as using the Lagrangian approach for mesh elements, or the same set of geometric points is followed through space (this is analogous to the material derivative).

Euler's first law of dynamics is chosen as governing equation for mesh motion

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{f}, \qquad (14)$$

where the integration limits are determined by spatial motion instead of physical motion (see figure 1). The total force $\boldsymbol{f}$ acting on a mesh element consists of two parts: a *body force* defined by

$$\boldsymbol{f}^b(t) = \int_{\boldsymbol{\xi}|_t(\Omega_{\boldsymbol{x}}^e)} \rho\breve{\boldsymbol{b}}\,\mathrm{d}V \qquad (15)$$

and a *contact force* governed by surface traction $\breve{\boldsymbol{T}}$

$$\boldsymbol{f}^c(t) = \int_{\boldsymbol{\xi}|_t(\partial\Omega_{\boldsymbol{x}}^e)} \breve{\boldsymbol{T}}\,\mathrm{d}A = \int_{\boldsymbol{\xi}|_t(\partial\Omega_{\boldsymbol{x}}^e)} \boldsymbol{n}\cdot\breve{\boldsymbol{\tau}}\,\mathrm{d}A. \qquad (16)$$

For equation $(16)_2$ it is assumed that Cauchy's theorem is valid for mesh motion (e.g. see I-Shih Liu [1]). Substitution of equations (13), (15) and (16) in Euler's first law (14) yields

$$\rho\frac{\partial\breve{\boldsymbol{v}}}{\partial t} = \nabla\cdot\breve{\boldsymbol{\tau}} + \rho\breve{\boldsymbol{b}}. \qquad (17)$$

This is essentially the equation of motion used in continuum mechanics, but it is here applied to govern mesh motion.

Any non-ideal physical phenomena (viz. irreversible) results in an amount of entropy production. This can be used to identify interesting regions in domains with physical (transport) phenomena. Regions with a higher entropy production probably require a refined mesh for a proper description. Starting with either a uniform mesh, for problems with no initial physical phenomena, or an adaptive mesh, for problems with initial physical phenomena, mesh motion can be governed by a spatial variation of entropy production.

The second law of thermodynamics can be written as localized master balance law (see also [12, 13])

$$\rho\mathcal{D}\hat{s} = -\nabla\cdot\boldsymbol{j}_S + \sigma_S, \qquad (18a)$$

where the volumetric rate of entropy production σ_S is always larger than zero

$$\sigma_S > 0, \qquad \forall\boldsymbol{y}\in\Omega_{\boldsymbol{y}}, t\in\mathbb{R}. \qquad (18b)$$

It will be shown how the volumetric rate of entropy production follows from the governing physical equations. This example also shows that a moving mesh does not result in additional entropy production.

Consider an arbitrary problem with transport phenomena governed by conservation of mass, linear momentum and total energy. Use the master balance law for specific internal energy $\hat{u}$ instead of the conservative law for total energy, so the problem is specified by (e.g. see Bird, Stewart and Lightfoot [14])

$$\mathcal{D}\rho = -\rho\nabla\cdot\boldsymbol{v}, \qquad (19)$$
$$\rho\mathcal{D}\boldsymbol{v} = -\nabla p + \nabla\cdot\boldsymbol{\tau}, \qquad (20)$$
$$\rho\mathcal{D}\hat{u} = -\nabla\cdot\boldsymbol{q} - p\nabla\cdot\boldsymbol{v} + \boldsymbol{\tau}:\nabla\otimes\boldsymbol{v}. \qquad (21)$$

By selecting this set of equations, the form for entropy flux $\boldsymbol{j}_S$ and volumetric rate of entropy production σ_S follow by thermodynamic considerations.

Combine the Gibbs relation for internal energy with the differential operator introduced in equation (7). Multiply by mass density ρ to get

$$\rho\mathcal{D}\hat{u} = \rho T\mathcal{D}\hat{s} - \rho p\mathcal{D}\hat{v}. \qquad (22)$$

Realise that $\rho\hat{v} = 1$, so the derivative of specific volume $\hat{v}$ can be written as

$$\rho\mathcal{D}\hat{v} = -\hat{v}\mathcal{D}\rho = \nabla\cdot\boldsymbol{v}, \qquad (23)$$

where continuity equation (19) is used. Substitution of equations (23), (21) and (18a) in the Gibbs relation yields

$$\begin{aligned} &-\nabla\cdot\boldsymbol{q} - p\nabla\cdot\boldsymbol{v} + \boldsymbol{\tau}:\nabla\otimes\boldsymbol{v} = \\ &\quad -T\nabla\cdot\boldsymbol{j}_S + T\sigma_S - p\nabla\cdot\boldsymbol{v}. \end{aligned} \qquad (24)$$

By solving for entropy flux and entropy production the following relations can be obtained

$$\boldsymbol{j}_S = -\frac{\boldsymbol{q}}{T}, \tag{25a}$$

$$\sigma_S = -\frac{\boldsymbol{q} \cdot \nabla T}{T^2} + \frac{\boldsymbol{\tau} : \nabla \otimes \boldsymbol{v}}{T}. \tag{25b}$$

Notice that mesh velocity does not appear in above terms, so governing mesh motion by the ALE formulation does not introduce additional entropy production.

The number of spatial dimensions of the calculation domain (n_{sd}) determines the number of PDEs for mesh motion (i.e. equation (17)). As stated before, spatial variation of the volumetric rate of entropy production will be used as driving force for mesh motion. Define the general form for body force density $\breve{\boldsymbol{b}}$ governing mesh motion as a multiplier times gradient of volumetric rate of entropy production, i.e.

$$\breve{\boldsymbol{b}} = \frac{\theta T}{\rho} \nabla \sigma_S. \tag{26}$$

A combination of a time constant θ, temperature T and mass density ρ is used as multiplier, because this yields consistent units for the equation of mesh motion. The time constant will be equal to one for all presented results and therefore omitted in the remainder of this paper. Since both temperature and mass density are always larger than zero, they do not disturb any direction dependence of the body force density.

One of the remaining issues is selecting the form for surface traction $\breve{\boldsymbol{T}}$. There are two approaches, which will result in different forms of the PDEs for mesh motion. Similar to elastic materials in solid mechanics, a stress-strain relation can be used. This approach will be called the mesh *displacement* method (MDM), since it yields a governing equation for mesh displacement. The second approach is based on an analogy to fluid mechanics, where a stress-strain rate relation is used for traction. Since this yields PDEs for mesh velocity, this will be called the mesh *velocity* method (MVM). Summarizing, the model for surface traction determines the final form of the moving mesh method:

$$\breve{\boldsymbol{T}}_{\text{MDM}} = \mathcal{T}(\nabla \otimes \breve{\boldsymbol{u}}), \tag{27}$$

$$\breve{\boldsymbol{T}}_{\text{MVM}} = \mathcal{T}(\nabla \otimes \breve{\boldsymbol{v}}). \tag{28}$$

Notice that this issue corresponds to determination of a constitutive relation (here for mesh motion), which explains the close resemblance of this work with thermoelasticity.

3.2 Mesh displacement method

Assume a mesh *behaves* like an isotropic, elastic material (e.g. rubber), so the analogy with continuum mechanics is further refined to solid mechanics. Mesh motion is determined in the form of mesh displacement, which is defined as function of (Cartesian) spatial coordinates and time by (see also figure 1)

$$\breve{\boldsymbol{u}}(\boldsymbol{y}, t) = \boldsymbol{y} - \boldsymbol{\xi}^{-1}(\boldsymbol{y}, t) \tag{29}$$

Mesh displacement could be defined by using referential coordinates, but since the master balance law is with respect to spatial coordinates above form is preferred. The current position of mesh vertices can be determined by above equation or by (numerical) integration of mesh velocity. Notice that mesh velocity has to be determined for evaluation of the convective velocity (see equation (7)).

In the classical theory of elasticity often the assumption is made that deformations are small, or

$$||\nabla \otimes \breve{\boldsymbol{u}}|| \ll 1. \tag{30}$$

This results in the following form for the (infinitesimal) strain tensor

$$\breve{\boldsymbol{e}} = \frac{1}{2}\left[\nabla \otimes \breve{\boldsymbol{u}} + (\nabla \otimes \breve{\boldsymbol{u}})^T\right]. \tag{31}$$

This assumption also allows to neglect the difference between the Cauchy and Piola-Kirchhoff stress tensors (see Salençon [3, p. 334-337]).

For a linear, elastic material, the (Cauchy) stress tensor $\boldsymbol{\tau}$ is modeled by the generalized Hooke's law

$$\tau_{ij} = \mathsf{c}_{ijkl} e_{kl}, \tag{32}$$

where c_{ijkl} is the elasticity tensor (4^{th} order). Above equation is only valid for homogeneous elastic constants (no dependence on position and time) and an initial stress-free and undeformed state. For an isotropic material the elastic constants can be specified by

$$\mathsf{c}_{ijkl} = \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl}, \tag{33}$$

where μ and λ are the Lamé moduli and δ_{ij} is the Kronecker delta.

Since traction is a function of mesh displacement, the time derivative of linear mesh momentum is written as second time derivative of mesh displacement. So the governing PDE(s) for the mesh displacement method yields

$$\rho\frac{\partial^2 \breve{\boldsymbol{u}}}{\partial t^2} - \nabla \cdot \left[2\mu\breve{\boldsymbol{e}} + \lambda(\text{tr}\,\breve{\boldsymbol{e}})\boldsymbol{\delta}\right] = T\nabla\sigma_S, \tag{34}$$

which is a wave equation with respect to the spatial coordinates. The Variational Arbitrary Lagrangian-Eulerian method presented by Thoutireddy [15] uses the same general form, but is evaluated for referential coordinates.

3.3 Mesh velocity method

The mesh velocity method (MVM) is a more straightforward implementation of the presented ideas. Basic assumption of the MVM is a diffusive character of mesh motion, where mesh motion is specified by mesh velocity. For a 1D problem, this assumption can be modeled by an analogy with Fourier's law for heat conduction

$$\breve{\tau} = -q = \breve{k}_{\text{MVM}} \frac{\partial \breve{v}}{\partial y}, \tag{35}$$

For multi-dimensional problems, a stress tensor analogous to an incompressible Newtonian fluid could be interesting, i.e.

$$\breve{\boldsymbol{\tau}} = \breve{k}_{\text{MVM}} \left[\nabla \otimes \breve{\boldsymbol{v}} + (\nabla \otimes \breve{\boldsymbol{v}})^T \right]. \tag{36}$$

Both analogies have only one parameter, which will be called mesh diffusivity $\breve{k}_{\text{MVM}}$.

Above analogy can be generalized to the following form of the governing PDE(s) for mesh motion

$$\rho \frac{\partial \breve{\boldsymbol{v}}}{\partial t} - \nabla \cdot \left\{ \breve{\mathbf{k}}_{\text{MVM}} \cdot \left[\nabla \otimes \breve{\boldsymbol{v}} + (\nabla \otimes \breve{\boldsymbol{v}})^T \right] \right\} = T \nabla \sigma_S, \tag{37}$$

where mesh diffusivity $\breve{\mathbf{k}}_{\text{MVM}}$ can be either a scalar or second order tensor (for an anisotropic mesh behaviour). Obviously, more elaborate models for surface traction can be selected as analogy, but this will introduce more mesh parameters.

An arbitrary moving boundary is implemented by specifying a Dirichlet boundary condition for mesh velocity

$$\breve{\boldsymbol{v}}(\boldsymbol{y}, t) = \breve{\boldsymbol{v}}_D(t), \quad \forall \boldsymbol{y} \in \left(\boldsymbol{\xi}|_t \left(\partial \Omega_{\boldsymbol{x}} \right) \right)_D. \tag{38}$$

An initial moving mesh is specified by a corresponding initial condition, or

$$\breve{\boldsymbol{v}}(\boldsymbol{y}, 0) = \breve{\boldsymbol{v}}_0(\boldsymbol{y}), \quad \forall \boldsymbol{y} \in \boldsymbol{\xi}|_t \left(\Omega_{\boldsymbol{x}} \right). \tag{39}$$

Mesh position is determined by an explicit algorithm

$$\boldsymbol{y}(t_{n+1}) = \boldsymbol{y}(t_n) + \int_{t_n}^{t_{n+1}} \breve{\boldsymbol{v}}(\tau) \, \mathrm{d}\tau. \tag{40}$$

Notice that since the equation of mesh motion solves for mesh velocity, the convective velocity can be determined directly.

4. NUMERICAL EXAMPLE

The feasibility of the suggested approach for a physical moving mesh will be shown by a numerical example. A rather artificial physical problem will be used to show some issues of the presented ideas. Assume a uniform, incompressible fluid flow in tube with constant cross-section. This problem can be modeled by the conservative law for total energy applied to a 1-dimensional geometry.

4.1 Problem statement

Governing PDE is the quasi-linear form of the energy balance, without mechanical work (stationary, incompressible, homogeneous flow, so there are no explicit terms for volume change and shear stresses)

$$\rho \, \hat{c}|_V \frac{\partial T}{\partial t} + \rho \, \hat{c}|_V \, (v - \breve{v}) \frac{\partial T}{\partial y} = -\frac{\partial q}{\partial y}, \tag{41}$$

which is equation (21) combined with the ideal gas equation of state. This equation has to be complemented by a constitutive relation for heat transfer, boundary conditions and initial conditions.

As constitutive relation for heat transfer due to conduction Fouries's law is applied (e.g. see Bird *et al* [14]),

$$q = -k \frac{\partial T}{\partial y} \tag{42}$$

It is assumed that the fluid enters the tube at a low temperature and exits at a higher temperature. This yields the following boundary conditions

$$T(0, t) = T_0, \qquad T(L, t) = T_0 + \Delta T, \tag{43}$$

with $\Delta T = 25 \ K$. An interesting initial condition is chosen, i.e.

$$T(y, 0) = T_0 + \frac{\Delta T}{2}, \qquad \forall y \in \Omega_{\boldsymbol{y}}. \tag{44}$$

This selection of boundary conditions and initial conditions results in two thermal boundary layers, where one of them will move through the domain due to convection of the fluid.

Nitrogen at standard conditions is selected as fluid ($p_0 = 1.013 \cdot 10^5 \ Pa$, $T_0 = 298.15 \ K$, source Yaws [16]), which has the following parameters

$$\begin{aligned} M &= 28.013 \ g \, mol^{-1}, \\ \rho &= 1.2498 \ kg \, m^{-3}, \\ k &= 0.02475 \ W \, m^{-1} \, K^{-1}, \\ \tilde{c}|_p &= 29.02 \ J \, mol^{-1} \, K^{-1}. \end{aligned}$$

Specific heat capacity at constant volume $\hat{c}|_V$ for an ideal gas yields then

$$\hat{c}|_V = \frac{\tilde{c}|_p - R}{M} = 0.7361 \ J \, kg^{-1} \, K^{-1}.$$

Default value for the fluid velocity is $v = 0.1 \ m \, s^{-1}$, so the problem is slightly convection-dominated.

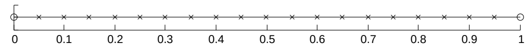

Figure 2: Default initial mesh for moving mesh method.

Overall length of the tube is $L = 1\ m$, which is spatially discretized into a uniform initial mesh (mesh size $h_x = 0.05\ m$, see figure 2). Fluid velocity determines the length of the time interval $t \in [0, 1/v]$. The non-stationary numerical solution approximates then the stationary solution of the problem (which is considered to be the equilibrium state). Default value for the time step $h_t = 0.01\ s$, but it depends on the selection of fluid velocity v and temperature difference ΔT between both boundaries.

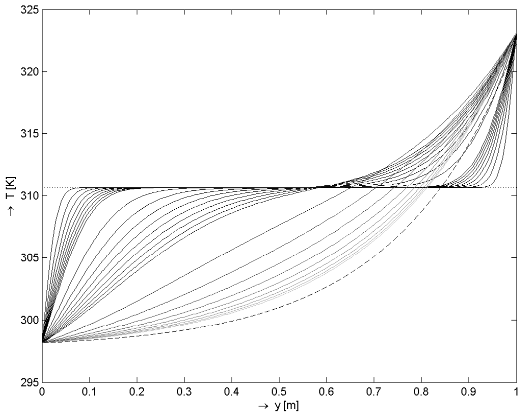

Figure 3: Numerical solution of temperature at various time steps ($t \in [0, 10]$) for a *fixed* mesh with default parameters. Dotted line shows initial condition and dashed line analytical solution of stationary problem.

Figure 3 shows the numerical solution of the specified problem on a fixed mesh. Though the problem is rather artificial, it is interesting since it has two thermal boundary layers. These boundary layers should be captured by the moving mesh, including the motion of the left boundary due to convection. When the left thermal boundary layer is merged with the right boundary layer, the steady state solution of equation (41) is reached (dashed line in figure 3). This can be considered as an equilibrium state, where the mesh should no longer move and should have reached an optimal configuration.

4.2 Physical moving mesh

Either equation (34) or equation (37) is used to govern mesh motion. This requires determination of the volumetric rate of entropy production due to irreversible heat transfer (see equation (25b)),

$$\sigma_S = -\frac{\boldsymbol{q} \cdot \nabla T}{T^2} \tag{45}$$

With substitution of Fourier's law, the gradient of the volumetric rate of entropy production due to heat transfer yields

$$\nabla \sigma_S = \nabla \left[\frac{k}{T^2} \nabla T \cdot \nabla T \right] \tag{46}$$

or, for Cartesian coordinates, in tensor notation

$$\frac{\partial \sigma_S}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{k}{T^2} \left(\frac{\partial T}{\partial x_j} \right)^2 \right]. \tag{47}$$

For a homogeneous and time independent thermal conductivity k this can be evaluated to

$$\frac{\partial \sigma_S}{\partial x_i} = \frac{2k}{T^2} \left[\frac{\partial T}{\partial x_j} \frac{\partial^2 T}{\partial x_i \partial x_j} - \frac{1}{T} \left(\frac{\partial T}{\partial x_j} \right)^2 \frac{\partial T}{\partial x_i} \right]. \tag{48}$$

Since a 1-dimensional geometry is used in this example, above equation yields the following form for the body force on mesh elements

$$\rho \breve{b} = T \frac{\partial \sigma_S}{\partial x} = \frac{2k}{T} \frac{\partial T}{\partial x} \left[\frac{\partial^2 T}{\partial x^2} - \frac{1}{T} \left(\frac{\partial T}{\partial x} \right)^2 \right]. \tag{49}$$

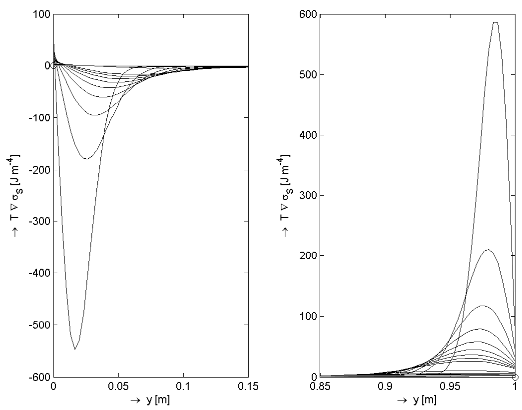

Figure 4: Body force on mesh elements based on entropy production near both boundaries at various time steps for a *fixed* mesh ($v = 0.1\ m\,s^{-1}$, $t \in [0, 10]$).

Time evaluation of body force on mesh elements on a fixed mesh is, for the specified problem, shown in figure 4. Due to the low value of (convective) fluid velocity with respect to the value for heat conductivity k, the figure is nearly point symmetric about the middle of the geometry.

Implementation of above equation is a bit tedious within the framework of FEMLAB® due to the second order spatial derivative of temperature. The general form of FEMLAB® implements a PDE as (e.g. see [17])

$$\boldsymbol{d}_\alpha \frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{\Gamma} = \boldsymbol{f}. \tag{50}$$

Gradient of the product of two scalars can be written as

$$\nabla (T \sigma_S) = T \nabla \sigma_S + \sigma_S \nabla T \tag{51}$$

and gradient of a scalar s can be written as a divergence by using the Kronecker delta $\boldsymbol{\delta}$

$$\nabla s = \nabla \cdot (s\boldsymbol{\delta}). \tag{52}$$

So the govern PDE for mesh motion becomes (for mesh velocity method)

$$\rho \frac{\partial \breve{\boldsymbol{v}}}{\partial t} + \nabla \cdot [-T\sigma_S \boldsymbol{\delta} - \breve{\boldsymbol{\tau}}] = -\sigma_S \nabla T. \tag{53}$$

This form is consistent with the general form of FEMLAB®. Notice that this equation couples mesh motion directly to irreversible physical phenomena.

4.3 Results

In this subsection various cases are evaluated of the same physical problem. Both the mesh displacement method and the mesh velocity method have a single parameter that determines the resistance to motion and deformation.

Mesh displacement method

The mesh displacement method (MDM) is based on similarities with the classical theory of linear elasticity. Due to the assumption made in equation (30), only small displacements are allowed. In order to get small values for the body force density, the temperature difference between both boundaries is set to $\Delta T = 2.5 \cdot 10^{-2}\ K$.

For a 1D geometry, the stress tensor $\breve{\tau}$ can be simplified to

$$\breve{\tau} = \breve{k}_{\mathrm{MDM}} \frac{\partial \breve{u}}{\partial y}. \tag{54}$$

Both material parameters λ and μ are combined in a single mesh parameter $\breve{k}_{\mathrm{MDM}}$.

Figure 5 shows the trajectory of the first interior vertex near both boundaries and the middle vertex (see figure 2 for mesh). The value of mesh parameter $\breve{k}_{\mathrm{MDM}}$ determines the behaviour of the mesh motion, since it determines the ratio of body force and surface traction. There are two modes of behaviour for mesh displacement.

The trajectory shown in figure 5 is obtained by using a small value for the mesh parameter ($\breve{k}_{\mathrm{MDM}} < 10^{-5}$). Mesh displacement has, initially, the same sign as body force density, so the direction of mesh motion is governed by irreversibilities. With increasing time, the trajectory begins to show a wave motion due to the increasing surface traction. For large values of the mesh parameter ($\breve{k}_{\mathrm{MDM}} \gg 10^{-5}$), surface traction is dominant and mesh displacement becomes uncontrolable.

Main objective of this implementation is to check whether the direction of mesh displacement corresponds with the sign of the gradient of the volumetric rate of entropy production. The suggested model for surface traction can not capture a time evolving solution. Because mesh displacement has to be small (due to equation (30)), the gradient can not change sufficiently. The restriction can be abolished by implementation of finite deformations and more elaborated forms of the stress tensor.

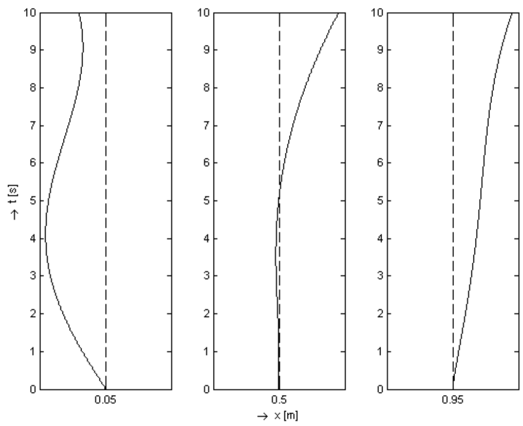

Figure 5: Trajectory of first, middle and last interior mesh vertex. Mesh motion is governed by mesh displacement method with $v = 0.1\ m\,s^{-1}$, $\Delta T = 2.5 \cdot 10^{-2}\ K$, $h_t = 0.005\ s$ and $\breve{k}_{\mathrm{MDM}} = 5 \cdot 10^{-6}\ J\,m^{-3}$.

Mesh velocity method

The mesh velocity method is an extension of the method suggested by the author for domains with moving boundaries ([9]). Similar problems arise again in this work. For a 1D geometry both models for traction are equal, yielding the following equation for mesh motion

$$\rho \frac{\partial \breve{v}}{\partial t} + \frac{\partial}{\partial y}\left[-\frac{k}{T}\left(\frac{\partial T}{\partial y}\right)^2 - \breve{k}_{\mathrm{MVM}} \frac{\partial \breve{v}}{\partial y}\right] = -\frac{k}{T^2}\left(\frac{\partial T}{\partial y}\right)^2 \frac{\partial T}{\partial y}, \tag{55}$$

where mesh diffusivity $\breve{k}_{\mathrm{MVM}}$ is the only parameter.

A low value for mesh diffusivity is required to make the moving mesh fast enough to capture the moving boundary layer. Figure 6 shows trajectories of mesh vertices for a low mesh diffusivity ($\breve{k}_{\mathrm{MVM}} = 0.25\ J\,s\,m^{-3}$). Vertices at the left boundary move to the left to capture the (thermal) boundary layer. The same phenomena occurs at the right boundary, where vertices are contracted to improve the description of the thermal boundary layer. After 1.5 s all vertices move to the right and follow more or less the moving left thermal boundary layer. Mesh motion seems to comply to the desired mesh motion, but it is still questionable whether the optimal mesh is obtained.

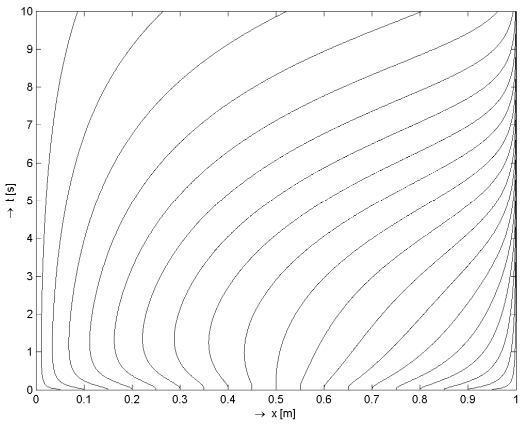

Figure 6: Trajectory of mesh vertices with mesh motion governed by the mesh velocity method. Parameters have default values, mesh diffusivity is $\breve{k}_{\mathrm{MVM}} = 0.25\ J\,s\,m^{-3}$.

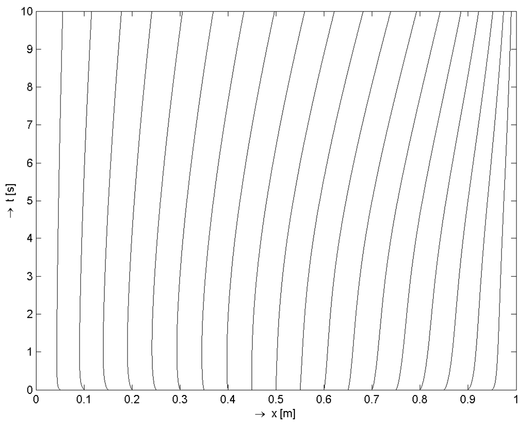

Figure 7: Trajectory of mesh vertices with mesh motion governed by the mesh velocity method. Parameters have default values, mesh diffusivity is $\breve{k}_{\mathrm{MVM}} = 2.5\ J\,s\,m^{-3}$.

One of the requirements for an optimal mesh would be a non-moving mesh when the equilibrium state is obtained. For the specified problem this means that the stationary solution (equilibrium state) has to be obtained after a surtain time. Evaluation of the problem for a long time interval yields problems near the right boundary. Too many vertices are contracted near the right boundary and some vertices move outside the calculation domain. These problems can be prevented by choosing a higher value for mesh diffusivity. Figure 7 shows trajectories of vertices for a higher value of mesh diffusivity. The overall behaviour is the same as for the lower mesh diffusivity, but it is less pronounced.

Mesh velocity method and prescribed moving boundary

As is already indicated in section 3.3, the mesh velocity method can be used for domains with moving boundaries. A moving boundary is implemented by specifying a non-homogeneous Dirichlet boundary condition, e.g.

$$\breve{v}(0,t) = 0, \quad \breve{v}(L,t) = \frac{A}{2}\sin(\omega t + \phi). \qquad (56)$$

Above boundary condition is combined with the specified physical problem, where the following parameters $A = 0.5\ m$, $\omega = v\pi\ Hz$ and $\phi = 0\ rad$ will be used.

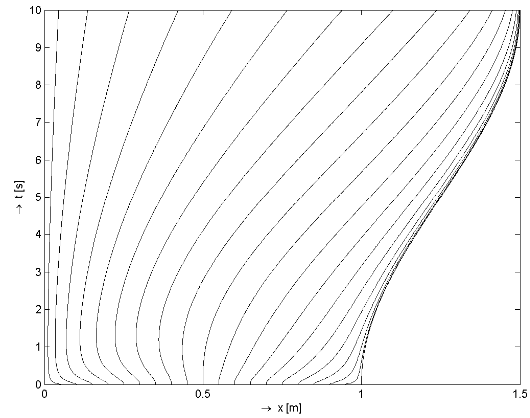

Figure 8: Trajectory of mesh vertices for $\breve{k}_{\mathrm{MVM}} = 0.25\ J\,s\,m^{-3}$, $v = 0.1\ m\,s^{-1}$ for a domain with a prescribed moving boundary. Mesh motion is governed by the mesh velocity method using entropy production as driving force.

Figure 8 shows the trajectories of mesh vertices when a moving mesh based on physics is used. The overall behaviour is similar to the solution with fixed boundaries. There seems to be less contraction of mesh vertices near the moving boundary (see also figure 6) and the vertices at the left boundary move not as fast as for the fixed boundary case.

It is interesting to compare the result of figure 8 with the method suggested by the author in earlier work ([9]). Figure 9 shows the trajectories when only the heat equation is used for mesh motion (viz. no coupling with physics). The same value for mesh diffusivity is used as in figure 8, which is sufficiently high to yield a sequence of solutions for the stationary Laplacian equation. This can be observed by the way all mesh vertices follow the moving boundary.

Stabilized mesh velocity method

For convective-dominated problems, the Galerkin method provides numerical instable solutions. There are various stabilization methods to overcome these instabilities. It will be shown that the suggested approach can be extended with stabilization methods known in the literature.

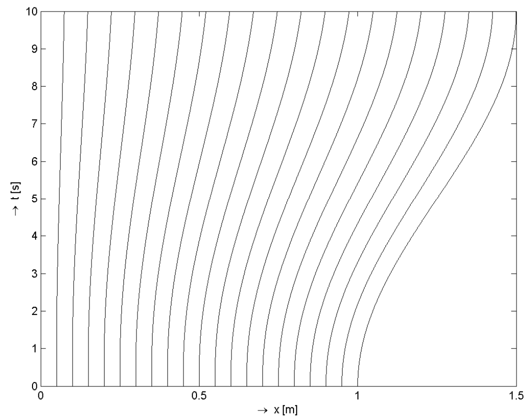

Figure 9: Trajectory of mesh vertices for $\breve{k}_{\text{MVM}} = 0.25\ J\,s\,m^{-3}$, $v = 0.1\ m\,s^{-1}$ for a domain with a prescribed moving boundary. Mesh motion is governed by the heat equation.

Numerical instabilities occur often at regions with a local (mesh) Péclet number larger than one, or

$$Pe = \frac{|\boldsymbol{v}|h_x}{2k} \leq 1. \tag{57}$$

For the specified problem ($h = 0.05$, $k = 0.02475$) the local Péclet number is almost equal to the convective velocity. Both convective velocity and mesh size can change due to a moving mesh, and in any combination of increasing or decreasing values. E.g., since some vertices move to the left in the example, the convective velocity increases and the mesh size decreases. It is not possible to predict how this effects the stability criterion for the local Péclet number.

Calculations are performed with high fluid velocities ($v = 100\ m\,s^{-1}$), which yield for a fixed mesh a numerical instable solution. The FEM-ALE approach is extended with the SUPG stabilization method ([18, 19]). The stabilized weak form for the *physical problem* yields, $\forall w^h \in \mathcal{V}^h$ find $u^h \in \mathcal{S}^h$ such that

$$\begin{aligned}
&\int_{\xi|_t(\Omega_x)} w^h \mathcal{D}\phi^h \,\mathrm{d}V + \\
&\quad\int_{\xi|_t(\Omega_x)} \nabla w^h \cdot \boldsymbol{j}|_\phi \,\mathrm{d}V + \\
&\quad\sum_{e=1}^{n_{el}} \int_{\xi|_t(\Omega_x^e)} \tau \mathcal{P} w^h \mathcal{R}\phi^h \,\mathrm{d}V = \\
&\quad\int_{\xi|_t(\Omega_x)} w^h \left[\sigma|_\phi - \phi^h(\nabla\cdot\boldsymbol{v})\right] \mathrm{d}V + \\
&\quad\int_{\xi|_t(\partial\Omega_x)} w^h\ h^h\Big|_\phi \,\mathrm{d}S.
\end{aligned} \tag{58}$$

Symbol n_{el} denotes the number of elements and Ω_x^e the domain corresponding with the e^{th} mesh element.

Differential operator $\mathcal{R}$ is the residual of the differential equation and perturbation operator $\mathcal{P}$, applied to the weight functions, is for the SUPG method specified by

$$\mathcal{P}w^h = (v - \breve{v})\nabla w^h. \tag{59}$$

Intrinsic time τ is according a paper of Tezduyar and Osawa [20]. Again, the difference between fluid velocity v and mesh velocity $\breve{v}$ is used as convective velocity. Intrinsic time has then the following form

$$\tau = \left(\frac{1}{\tau_{S1}^r} + \frac{1}{\tau_{S2}^r} + \frac{1}{\tau_{S3}^r}\right)^{-1/r} \tag{60}$$

with

$$\tau_{S1} = \frac{h_x}{2|v - \breve{v}|}, \quad \tau_{S2} = \frac{h_t}{2}, \quad \tau_{S3} = \frac{h_x^2}{4k}. \tag{61}$$

Only the equation for the physical problem is extended with stabilization method. This extension shows numerical stable solutions for high fluid velocities, where the results are similar to figure 3 (though the time interval is shorter). The drawback is the requirement of a higher value for mesh diffusivity (i.e. $\breve{k} = 2$ for this example), which yields a less flexible moving mesh.

5. CONCLUSION

Objective of this paper is to present the concept of a moving mesh method with mesh motion governed by entropy production. The paper shows that the concept is feasible, but it also shows that there remain issues to be solved. The suggested method is capable of responding to the governing physics *and* can be applied to a domain with arbitrary moving boundaries.

One of the main issues is the actual form for surface traction in the governing equation for mesh motion. Using a single, constant parameter to govern the behaviour of the mesh is not sufficient generic for all cases. The mesh parameter or diffusivity should depend at least of the mesh size, so there is a higher resistance to deformation near a boundary layer. A more advanced form of surface traction should yield a non-moving, optimal mesh when the equilibrium state is obtained and include a mechanism to control mesh quality. This prevents collapsing of elements or vertices moving outside the calculation domain.

Another issue is to determine how the suggested method should be extended with stabilization methods. The paper shows that a straightforward implementation of existing methods is feasible if the difference between fluid velocity and mesh velocity is used as convective velocity. Due to the moving mesh, all stability criteria have to be analysed for required modifications (local mesh Péclet number, Courant-Friedrichs-Lewy number). It could be interesting to extend the PDE(s) for mesh motion with a stabilization method.

The paper is restricted to a single physical phenomena (heat conduction). A combination of physical phenomena (i.e. dynamic fluid flow, diffusion, chemical reactions, ...) should be implemented to see how they interact. These issues will be studied more elaborately in the continuation of this research project.

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