Term Project/Semesterarbeit

(Computational Science & Engineering)

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Numerical Simulation of Harmonic Map Heat Flow

1 Governing equations

Harmonic map heat flow refers to the gradient flow of the Dirichlet functional for vector fields of unit length. On a given computational domain $\Omega \subset \mathbb{R}^2$ and for a given period of time $]0,T[$, $T > 0$, this results in the evolution equations for $\mathbf{m} = \mathbf{m}(t,\mathbf{x}) :]0,T[\times\Omega \mapsto \mathbb{R}^3$:

$$\begin{aligned} \frac{\partial \mathbf{m}}{\partial t} &= \mathbf{m} \times (\Delta \mathbf{m} \times \mathbf{m}) \quad \text{in }]0,T[\times\Omega\,, \\ \mathbf{m}(0) &= \mathbf{m}_0 \quad \text{in } \Omega\,, \\ \frac{\partial \mathbf{m}}{\partial \mathbf{n}} &= 0 \quad \text{on }]0,T[\times\partial\Omega\,. \end{aligned} \tag{1}$$

The underlying energy is

$$\mathcal{E}(\mathbf{m}) = \tfrac{1}{2}\int_\Omega |\nabla \mathbf{m}|^2 \,\mathrm{d}\mathbf{x}\,, \tag{2}$$

where $\nabla \mathbf{m}$ designates the Jacobi matrix of $\mathbf{m}$ and $|\nabla \mathbf{m}|$ gives its Frobenius norm. Thanks to the boundary condition on $\mathbf{m}$, we find

$$\begin{aligned} \frac{d\mathcal{E}(\mathbf{m})}{dt} &= \int_\Omega \nabla \mathbf{m} : \nabla \frac{\partial \mathbf{m}}{\partial t}\,\mathrm{d}\mathbf{x} = -\int_\Omega \Delta \mathbf{m} \cdot \frac{\partial \mathbf{m}}{\partial t}\,\mathrm{d}\mathbf{x} \\ &= -\int_\Omega \Delta \mathbf{m} \cdot (\mathbf{m} \times (\Delta \mathbf{m} \times \mathbf{m}))\,\mathrm{d}\mathbf{x} = -\int_\Omega |\Delta \mathbf{m} \times \mathbf{m}|^2\,\mathrm{d}\mathbf{x} \end{aligned} \tag{3}$$

This reveals that harmonic map heat flow is a dissipative process with respect to the energy from (2). Moreover,

$$\frac{d|\mathbf{m}|^2}{dt} = 2\mathbf{m} \cdot \frac{\partial \mathbf{m}}{\partial t} = 2\mathbf{m} \cdot (\mathbf{m} \times (\Delta \mathbf{m} \times \mathbf{m})) = 0\,,$$

which shows that $|\mathbf{m}(t,\mathbf{x})| = |\mathbf{m}_0(\mathbf{x})|$ for all $(t,\mathbf{x}) =]0,T[\times\Omega$. If we fix $|\mathbf{m}_0| = 1$ almost erverywhere in Ω, which is usually done, then $|\mathbf{m}| = 1$ almost everywhere for all times.

In the sequel, let us assume that $|\mathbf{m}(t,\mathbf{x})| = 1$ for all $(t,\mathbf{x}) =]0,T[\times\Omega$ ("saturation"). Moreover, recall the identity

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b}) \quad \forall \mathbf{a},\mathbf{b},\mathbf{c}\in\mathbb{R}^3 \; . \tag{4}$$

This implies

$$\mathbf{m}\times(\Delta\mathbf{m}\times\mathbf{m}) = \Delta\mathbf{m} - \mathbf{m}(\Delta\mathbf{m}\cdot\mathbf{m}) \; . \tag{5}$$

2 Timestepping

For the temporal discretization of (1) the method of Heun can be employed. We use an equidistant grid in time and try to compute $\mathbf{m}(t)$ for instances $t_n := nk$, $k = {}^{T}/{}_{M}$. We introduce the notations

$$\mathbf{m}^n \approx \mathbf{m}(t_n) \quad , \quad \delta_t\mathbf{m}^{n+1/2} \approx \frac{\mathbf{m}^{n+1}-\mathbf{m}^n}{k} \quad , \quad \overline{\mathbf{m}}^{n+1/2} \approx \tfrac{1}{2}(\mathbf{m}^{n+1}-\mathbf{m}^n) \; .$$

Then the discrete evolution can be stated as

$$\delta_t\mathbf{m}^{n+1/2} = \overline{\mathbf{m}}^{n+1/2}\times(\Delta\overline{\mathbf{m}}^{n+1/2}\times\overline{\mathbf{m}}^{n+1/2}) \; , \quad \mathbf{m}^0 = \mathbf{m}_0 \quad \text{in } \Omega \; . \tag{6}$$

Multiplying (6) with $\overline{\mathbf{m}}^{n+1/2}$ we find

$$|\mathbf{m}^{n+1}|^2 - |\mathbf{m}^n|^2 = 0 \quad \Rightarrow \quad |\mathbf{m}^n| = |\mathbf{m}_0| \quad \forall n \; , \tag{7}$$

which means that the conservation of modulus carries over to the semi-discrete problem (6). Further,

$$\begin{aligned}\mathcal{E}(\mathbf{m}^{n+1}) - \mathcal{E}(\mathbf{m}^n) &= \tfrac{1}{2}\int_\Omega (\nabla\mathbf{m}^{n+1}+\nabla\mathbf{m}^n) : (\nabla\mathbf{m}^{n+1}-\nabla\mathbf{m}^n)\,\mathrm{d}\mathbf{x} \\ &= -k\int_\Omega \Delta\overline{\mathbf{m}}^{n+1/2}\cdot\delta_t\mathbf{m}^{n+1/2} \\ &= -k\int_\Omega \Delta\overline{\mathbf{m}}^{n+1/2}\cdot\Big(\overline{\mathbf{m}}^{n+1/2}\times(\Delta\overline{\mathbf{m}}^{n+1/2}\times\overline{\mathbf{m}}^{n+1/2})\Big)\,\mathrm{d}\mathbf{x} \\ &= -k\int_\Omega |\Delta\overline{\mathbf{m}}^{n+1/2}\times\overline{\mathbf{m}}^{n+1/2}|^2\,\mathrm{d}\mathbf{x} \; .\end{aligned} \tag{8}$$

3 Mixed variational formulation

Let us focus on the problem to be solved in each timestep of (6): introducing new unknown $\mathbf{j} := \nabla\overline{\mathbf{m}^{n+1/2}}$ we end up with

$$\begin{aligned}\delta_t\mathbf{m}^{n+1/2} &= \overline{\mathbf{m}}^{n+1/2}\times(\operatorname{div}\overline{\mathbf{j}}^{n+1/2}\times\overline{\mathbf{m}}^{n+1/2}) \; , \\ \mathbf{j}^n &= \nabla\overline{\mathbf{m}}^n \; .\end{aligned}$$

These equations can be cast in weak form: seek $\mathbf{m}^{n+1} \in (L^2(\Omega))^3 \cap L^\infty(\Omega)^3$ and $\mathbf{j}^{n+1} \in (\boldsymbol{H}_0(\mathrm{div};\Omega))^3$ such that

$$\begin{aligned} \left(\delta_t \mathbf{m}^{n+1/2}, \mathbf{v}\right)_0 &= \left(\mathrm{div}\,\overline{\mathbf{j}}^{n+1/2} \times \overline{\mathbf{m}}^{n+1/2}, \mathbf{v} \times \overline{\mathbf{m}}^{n+1/2}\right)_0 \quad \forall \mathbf{v} \in (L^2(\Omega))^3 \;, \\ \left(\mathbf{j}^{n+1}, \mathbf{q}\right)_0 + \left(\mathrm{div}\,\mathbf{q}, \mathbf{m}^{n+1}\right)_0 &= 0 \quad \forall \mathbf{q} \in (\boldsymbol{H}_0(\mathrm{div};\Omega))^3 \;. \end{aligned} \tag{9}$$

Now, let us consider an abstract spatial Galerkin discretization based on the finite-dimensional spaces $Q_h \subset (L^2(\Omega))^3$, $\mathbf{v}_h \in (\boldsymbol{H}_0(\mathrm{div};\Omega))^3$: seek $\mathbf{m}_h^{n+1} \in Q_h$, $\mathbf{j}_h^{n+1} \in \mathbf{V}_h$ such that

$$\begin{array}{rcccl} \left(\delta_t \mathbf{m}_h^{n+1/2}, \mathbf{v}_h\right)_0 & - & \left(\mathrm{div}\,\overline{\mathbf{j}}^{n+1/2} \times \overline{\mathbf{m}}_h^{n+1/2}, \mathbf{v} \times \overline{\mathbf{m}}_h^{n+1/2}\right)_0 & = & 0 \quad \forall \mathbf{v}_h \in Q_h \;, \\ \left(\mathrm{div}\,\mathbf{q}_h, \mathbf{m}_h^{n+1}\right)_0 & + & \left(\mathbf{j}_h^{n+1}, \mathbf{q}_h\right)_0 & = & 0 \quad \forall \mathbf{q}_h \in \mathbf{V}_h \;. \end{array} \tag{10}$$

The discrete energy at time t_n is given by

$$\mathcal{E}_n := \tfrac{1}{2} \int_\Omega |\mathbf{j}_h^n|^2 \,\mathrm{d}\mathbf{x} \;. \tag{11}$$

It decays according to

$$\begin{aligned} \mathcal{E}_{n+1} - \mathcal{E}_n &= \tfrac{1}{2} \int_\Omega |\mathbf{j}_h^{n+1}|^2 - |\mathbf{j}_h^n|^2 \,\mathrm{d}\mathbf{x} = \tfrac{1}{2} \left(\mathbf{j}_h^{n+1} + \mathbf{j}_h^n, \mathbf{j}_h^{n+1} - \mathbf{j}_h^n\right)_0 \\ &= \left(\mathbf{j}_h^{n+1} - \mathbf{j}_h^n, \overline{\mathbf{j}}_h^{n+1/2}\right)_0 = -k \left(\mathrm{div}\,\overline{\mathbf{j}}_h^{n+1/2}, \delta_t \mathbf{m}^{n+1/2}\right)_0 \\ &= -k \left\| \mathrm{div}\,\overline{\mathbf{j}}_h^{n+1/2} \times \overline{\mathbf{m}}_h^{n+1/2} \right\|_{L^2(\Omega)}^2 \;. \end{aligned}$$

So, regardless of the Galerkin spaces chosen, we obtain a stable method.

Remark. We may use (5) in order to recast (10) as

$$\begin{array}{rcccccl} \left(\delta_t \mathbf{m}_h^{n+1/2}, \mathbf{v}_h\right)_0 & - & \left(\mathrm{div}\,\overline{\mathbf{j}}^{n+1/2}, \mathbf{v}_h\right)_0 & = & \left(\mathrm{div}\,\overline{\mathbf{j}}^{n+1/2} \cdot \overline{\mathbf{m}}_h^{n+1/2}, \overline{\mathbf{m}}_h^{n+1/2} \cdot \mathbf{v}_h\right)_0 & \forall \mathbf{v}_h \in Q_h \;, \\ \left(\mathrm{div}\,\mathbf{q}_h, \mathbf{m}_h^{n+1}\right)_0 & + & \left(\mathbf{j}_h^{n+1}, \mathbf{q}_h\right)_0 & = & 0 & \forall \mathbf{q}_h \in \mathbf{V}_h \;. \end{array} \tag{12}$$

4 Finite element Galerkin discretization

We assume that Ω is covered by a triangular mesh $\mathcal{M}$. The following conforming finite element trial spaces will be employed:

for $(L^2(\Omega))^3$: space of $\mathcal{M}$-piecewise constant vectorfields on Ω,
for $\boldsymbol{H}(\mathrm{div};\Omega)$: lowest order Raviart-Thomas finite element space

The local shape functions for the Raviart-Thomas finite element space on a triangle with vertices $\mathbf{a}^1, \mathbf{a}^2, \mathbf{a}^3$ are given by

$$\mathbf{b}_i(\mathbf{x}) = \frac{|e_i|}{2|T|} (\mathbf{x} - \mathbf{a}_i) \cdot \mathbf{n}_i \;, \tag{13}$$

where e_i is the edge opposite to the vertes $\mathbf{a}_i$ and $\mathbf{n}_i$ designates the exterior unit normal vector to that edge. These local shape functions are dual to the local degrees of freedom:

$$\int_{e_j} \mathbf{b} \cdot \mathbf{n}_j \, \mathrm{d}S = \delta_{ij} \;, \quad i,j = 1,2,3 \;. \tag{14}$$

Using the canonical global shape functions for these finite element spaces, (9) is converted into a non-limnear system of equations. It can be solved using Newton's iteration with the solutions from the previous time-step as initial guesses.

Task. Implementation of the numerical method described above and detailed studies of stability and convergence with respect to variation of spatial and temporal resolution. Parallelization on a Linux cluster.

Focus. Implementation and analysis of a finite element scheme.

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