Contents

1 Frank Oseen energy

In $\mathbb{R}^3$:

$$E_{\text{FO}} = \frac{1}{2}\int_\Omega K_1 \left(\nabla\cdot\mathbf{p}\right)^2 + K_2\left(\mathbf{p}\cdot[\nabla\times\mathbf{p}]\right)^2 + K_3\left\|\mathbf{p}\times[\nabla\times\mathbf{p}]\right\|^2 dV \tag{1}$$

With the Langrange identity for the K_3-term, we cann rewrite (1) to

$$E_{\text{FO}} = \frac{1}{2}\int_\Omega K_1 \left(\nabla\cdot\mathbf{p}\right)^2 + (K_2 - K_3)\left(\mathbf{p}\cdot[\nabla\times\mathbf{p}]\right)^2 + K_3\left\|\mathbf{p}\right\|^2\left\|\nabla\times\mathbf{p}\right\|^2 dV \tag{2}$$

If we restrict (2) to a 2-dimensional Manifold $M\subset\Omega$ and postulate that $\mathbf{p}\in T_XM$ is a normalized tangential vector in $X\in M$, we get

$$E_{\text{FO}} = \frac{1}{2}\int_M K_1\left(\mathrm{Div}\mathbf{p}\right)^2 + K_3\left(\mathrm{Rot}\mathbf{p}\right)^2 dA \tag{3}$$

In terms of exterior calculus with the corresponding 1-form $\mathbf{p}^\flat\in\Lambda^1(M)$, ,i.e. $\left(\mathbf{p}^\flat\right)^\sharp = \mathbf{p}$, we obtain

$$E_{\text{FO}} = \frac{1}{2}\int_M K_1\left(\mathbf{d}^*\mathbf{p}^\flat\right)^2 + K_3\left(*\mathbf{d}\mathbf{p}^\flat\right)^2 dA \tag{4}$$

where the exterior coderivative $\mathbf{d}^* := -*\mathbf{d}*$ is the L^2-orthogonal operator of the exterior derivative $\mathbf{d}$. (Note $\mathrm{Div}\mathbf{p} = -\mathbf{d}^*\mathbf{p}^\flat$ and $\mathrm{Rot}\mathbf{p} = *\mathbf{d}\mathbf{p}^\flat$)

1.1 Functional derivative

With the L^2-orthogonality of the exterior derivative and coderivative ($\langle \mathbf{d}\bullet,\bullet\rangle_{L^2} = \langle \bullet, \mathbf{d}^*\bullet\rangle_{L^2}$) and a arbitrary $\alpha \in \Lambda^1(M)$ we get

$$\int_M \left\langle \frac{\delta E_{\mathrm{FO}}}{\delta \mathbf{p}^\flat}, \alpha \right\rangle dA = \lim_{\epsilon\to 0} \frac{1}{\epsilon} \left(E_{\mathrm{FO}} \left[\mathbf{p}^\flat + \epsilon\alpha\right] - E_{\mathrm{FO}} \left[\mathbf{p}^\flat\right] \right) \tag{5}$$

$$= \lim_{\epsilon\to 0} \frac{1}{2\epsilon} \int_M K_1 \left(2\epsilon \left(\mathbf{d}^*\mathbf{p}^\flat\right)(\mathbf{d}^*\alpha) + \epsilon^2 (\mathbf{d}^*\alpha)^2 \right) \tag{6}$$

$$+ K_3 \left(2\epsilon \left\langle \mathbf{d}\mathbf{p}^\flat, \mathbf{d}\alpha \right\rangle + \epsilon^2 \|\mathbf{d}\alpha\|^2 \right) dA \tag{7}$$

$$= -\int_M K_1 \left\langle \mathbf{\Delta}^{\mathrm{GD}}\mathbf{p}^\flat, \alpha \right\rangle + K_3 \left\langle \mathbf{\Delta}^{\mathrm{RR}}\mathbf{p}^\flat, \alpha \right\rangle dA \tag{8}$$

$$= \int_M \left\langle -\left(K_1\mathbf{\Delta}^{\mathrm{GD}} + K_3\mathbf{\Delta}^{\mathrm{RR}}\right)\mathbf{p}^\flat, \alpha \right\rangle dA \tag{9}$$

where $\mathbf{\Delta}^{\mathrm{RR}} = -\mathbf{d}^*\mathbf{d} = *\mathbf{d}*\mathbf{d}$ is the Vector-Laplace-Beltrami-Operator or Rot-Rot-Laplace and $\mathbf{\Delta}^{\mathrm{GD}} = -\mathbf{d}\mathbf{d}^* = \mathbf{d}*\mathbf{d}*$ is the Vector-Laplace-CoBeltrami-Operator or Grad-Div-Laplace. Hence, for a One-Constant-Approximation $K_1 = K_3 =: K_0$, we obtain

$$\int_M \left\langle \frac{\delta E_{\mathrm{FO}}}{\delta \mathbf{p}^\flat}, \alpha \right\rangle dA = \int_M \left\langle K_0 \mathbf{\Delta}^{\mathrm{dR}}\mathbf{p}^\flat, \alpha \right\rangle dA \tag{10}$$

where $\mathbf{\Delta}^{\mathrm{dR}} = -\mathbf{\Delta}^{\mathrm{RR}} - \mathbf{\Delta}^{\mathrm{GD}} = \mathbf{d}^*\mathbf{d} + \mathbf{d}\mathbf{d}^*$ is the Laplace-de Rham operator.

1.2 Unit vector invariance

If $\mathbf{p} \in T_X M$ is a unit vector on M, we can describe all unit vectors in $X \in M$ as a rotation in the tangential space with angle $\phi \in \mathbb{R}$:

$$\mathbf{q} = \cos\phi\mathbf{p} + \sin\phi\,(*\mathbf{p}) \tag{11}$$

$*\mathbf{p} = \left(*\mathbf{p}^\flat\right)^\sharp$ is the Hodge dual of $\mathbf{p}$, i.e. a quarter rotation of $\mathbf{p}$. For a space independent angle ϕ, i.e. $\mathbf{d}\phi = 0$, straight forward calculations implies

$$\|\mathrm{Rot}(*\mathbf{p})\| = \left\| *\mathbf{d} * \mathbf{p}^\flat \right\| = \|\mathrm{Div}\mathbf{p}\| \tag{12}$$

$$\|\mathrm{Div}(*\mathbf{p})\| = \left\| *\mathbf{d} * *\mathbf{p}^\flat \right\| = \left\| *\mathbf{d}\mathbf{p}^\flat \right\| = \|\mathrm{Rot}\mathbf{p}\| \tag{13}$$

$$\|\mathrm{Rot}\mathbf{q}\|^2 = \left\| *\mathbf{d}\mathbf{q}^\flat \right\|^2 = \left\| \mathbf{d}\mathbf{q}^\flat \right\|^2 \tag{14}$$

$$= \cos^2\phi\,\|\mathrm{Rot}\mathbf{p}\|^2 + \sin^2\phi\,\|\mathrm{Div}\mathbf{p}\|^2 + 2\cos\phi\sin\phi \left\langle \mathbf{d}\mathbf{p}^\flat, \mathbf{d} * \mathbf{p}^\flat \right\rangle \tag{15}$$

$$\|\mathrm{Div}\mathbf{q}\|^2 = \left\| *\mathbf{d} * \mathbf{q}^\flat \right\|^2 = \left\| \mathbf{d} * \mathbf{q}^\flat \right\|^2 \tag{16}$$

$$= \cos^2\phi\,\|\mathrm{Div}\mathbf{p}\|^2 + \sin^2\phi\,\|\mathrm{Rot}\mathbf{p}\|^2 - 2\cos\phi\sin\phi \left\langle \mathbf{d}\mathbf{p}^\flat, \mathbf{d} * \mathbf{p}^\flat \right\rangle \tag{17}$$

Finally, we get for the One-Constant-Approximation of the Frank-Oseen-Energy

$$E_{\mathrm{FO}}[\mathbf{q}] = E_{\mathrm{FO}}[\mathbf{p}] \tag{18}$$

2 Normalizing energy

To constrain $\mathbf{p}$ is normalized, we add

$$E_n = \int_M \frac{K_n}{4} \left(\|\mathbf{p}\|^2 - 1 \right)^2 dA \tag{19}$$

to the Frank Oseen energy. Note that the norm defined by the metric g on the manifold M is invariant regarding lowering or rising the indices, i.e.

$$\|\mathbf{p}\|^2 = p^i g_{ij} p^j = p_i g^{ij} p_j = \left\|\mathbf{p}^\flat\right\|^2 \tag{20}$$

2.1 Functional derivative

By variating $\mathbf{p}^\flat$ under the norm with an arbitrary $\alpha \in \Lambda^1(M)$, we obtain

$$\left\|\mathbf{p}^\flat + \epsilon\alpha\right\|^2 = \left\|\mathbf{p}^\flat\right\|^2 + 2\epsilon\left\langle \mathbf{p}^\flat, \alpha\right\rangle + \epsilon^2 \|\alpha\|^2 \tag{21}$$

If we are only interesting in linear terms (in ϵ), this leads to

$$\left(\left\|\mathbf{p}^\flat + \epsilon\alpha\right\|^2 - 1\right)^2 = \left(\left\|\mathbf{p}^\flat\right\|^2 - 1 + 2\epsilon\left\langle \mathbf{p}^\flat, \alpha\right\rangle + \mathcal{O}\left(\epsilon^2\right)\right)^2 \tag{22}$$

$$= \left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)^2 + 4\epsilon\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)\left\langle \mathbf{p}^\flat, \alpha\right\rangle + \mathcal{O}\left(\epsilon^2\right) \tag{23}$$

Hence, we get for the functional derivative of E_n

$$\int_M \left\langle \frac{\delta E_n}{\delta \mathbf{p}^\flat}, \alpha \right\rangle dA = \lim_{\epsilon\to 0} \frac{1}{\epsilon}\left(E_n\left[\mathbf{p}^\flat + \epsilon\alpha\right] - E_n\left[\mathbf{p}^\flat\right]\right) \tag{24}$$

$$= \int_M \left\langle K_n\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)\mathbf{p}^\flat, \alpha\right\rangle dA \tag{25}$$

3 Model equations

To minimize the energy $E := E_{\mathrm{FO}} + E_n$ we choose a time evolving approach. Hence, with the fundamental lemma of calculus of variations, we will use the time depended differential equation in terms of exterior calculus

$$\partial_t \mathbf{p}^\flat = -\frac{\delta E}{\delta \mathbf{p}^\flat} = -K_0 \mathbf{\Delta}^{\mathrm{dR}} \mathbf{p}^\flat - K_n\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)\mathbf{p}^\flat \tag{26}$$

or in general, if we don't want to use the One-Constant-Approximation,

$$\partial_t \mathbf{p}^\flat = \left(K_1 \mathbf{\Delta}^{\mathrm{GD}} + K_3 \mathbf{\Delta}^{\mathrm{RR}}\right)\mathbf{p}^\flat - K_n\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)\mathbf{p}^\flat \tag{27}$$

Note that if we apply the Hodge operator on the whole equations, we get the Hodge dual equations

$$\partial_t(*\mathbf{p}^\flat) = -K_0 \mathbf{\Delta}^{\mathrm{dR}}(*\mathbf{p}^\flat) - K_n\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)(*\mathbf{p}^\flat) \tag{28}$$

$$= \left(K_1 \mathbf{\Delta}^{\mathrm{RR}} + K_3 \mathbf{\Delta}^{\mathrm{GD}}\right)(*\mathbf{p}^\flat) - K_n\left(\left\|\mathbf{p}^\flat\right\|^2 - 1\right)(*\mathbf{p}^\flat) \tag{29}$$

which are very useful for the DEC discretization later in context. But this leads to pay attention, because only in the first line (One-Constant-Approximation) we see, that the Hodge dual equations in $*\mathbf{p}^\flat$ is the same as the primal equation in $\mathbf{p}^\flat$. In the general case (second line), we must "swap" the Laplace operators.

4 Needed DEC stuff

For further information see for example [Whi57, Hir03].

4.1 Surface Mesh

...wellcentered manifoldlike simplicial complex, bla, bla, blub...

4.2 Discrete 1-forms

The main concept to represent a discrete 1-form $\mathbf{p}_h^\flat \in \Lambda_h^1(K)$ is to approximate the contraction of the continuous 1-Form $\mathbf{p}^\flat \in \Lambda^1(M)$ on all edges $e \in \mathcal{E}$

$$\mathbf{p}_h^\flat(e) := \int_{\pi(e)} \mathbf{p}^\flat \approx \int_0^1 \mathbf{p}^\flat_{X_e(\tau)} \left(\dot{X}_e(t)\right) dt = \mathbf{p}^\flat_{X_e(\tau)}(\mathbf{e}) \tag{30}$$

where $\pi : K \to M$ is the glueing map, who project the elements of the surface mesh to the manifold. $X_e(t) = t\mathbf{v}_2 + (1-t)\mathbf{v}_1$ is the linear barycentric parametrisation of the edge $e = [v_1, v_2]$. The existence of a intermediate value $\tau \in [0,1]$, so that $\mathbf{e} \in T_{X_e(\tau)}M$, is ensured by the mean value theorem. Other discrete forms of arbitrary degree and theirs hodge duals can be interpreted in a similarly way.

4.3 Discrete Laplace operators

In the discrete exterior calculus discrete Operators are defined by successively interpretation of the basic operations on the forms, like the Hodge operator $*$ or the exterior derivative $\mathbf{d}$, as geometric operators on the simplices, like the Voronoi dual operator $\star$ or the boundary operator ∂ (see [Hir03]). This results for example to a discrete definition of $\mathbf{\Delta}^{\mathrm{RR}}$ for a discrete 1-form $\mathbf{p}_h^\flat \in \Lambda_h^1(M)$ on a edge $e \in \mathcal{E}$

$$\mathbf{\Delta}_h^{\mathrm{RR}}\mathbf{p}_h^\flat(e) := \left(*\mathbf{d}*\mathbf{d}\mathbf{p}_h^\flat\right)(e) = -\frac{|e|}{|\star e|}\left(\mathbf{d}*\mathbf{d}\mathbf{p}_h^\flat\right)(\star e) \tag{31}$$

$$= -\frac{|e|}{|\star e|}\left(*\mathbf{d}\mathbf{p}_h^\flat\right)(\partial \star e) = -\frac{|e|}{|\star e|}\sum_{f \succ e} s_{f,e}\left(*\mathbf{d}\mathbf{p}_h^\flat\right)(\star f) \tag{32}$$

$$= -\frac{|e|}{|\star e|}\sum_{f \succ e}\frac{s_{f,e}}{|f|}\left(\mathbf{d}\mathbf{p}_h^\flat\right)(f) = -\frac{|e|}{|\star e|}\sum_{f \succ e}\frac{s_{f,e}}{|f|}\mathbf{p}_h^\flat(\partial f) \tag{33}$$

$$= -\frac{|e|}{|\star e|}\sum_{f \succ e}\frac{s_{f,e}}{|f|}\sum_{\tilde{e} \prec f} s_{f,\tilde{e}}\mathbf{p}_h^\flat(\tilde{e}) \tag{34}$$

or for $\mathbf{\Delta}^{\mathrm{GD}}$

$$\mathbf{\Delta}_h^{\mathrm{GD}}\mathbf{p}_h^\flat(e) := \left(\mathbf{d}*\mathbf{d}*\mathbf{p}_h^\flat\right)(e) = \left(*\mathbf{d}*\mathbf{p}_h^\flat\right)(\partial e) \tag{35}$$

$$= \sum_{v \prec e} s_{v,e}\left(*\mathbf{d}*\mathbf{p}_h^\flat\right)(v) = \sum_{v \prec e}\frac{s_{v,e}}{|\star v|}\left(\mathbf{d}*\mathbf{p}_h^\flat\right)(\star v) \tag{36}$$

$$= \sum_{v \prec e}\frac{s_{v,e}}{|\star v|}\left(*\mathbf{p}_h^\flat\right)(\partial \star v) = -\sum_{v \prec e}\frac{s_{v,e}}{|\star v|}\sum_{\tilde{e} \succ v} s_{v,\tilde{e}}\left(*\mathbf{p}_h^\flat\right)(\star\tilde{e}) \tag{37}$$

$$= -\sum_{v \prec e}\frac{s_{v,e}}{|\star v|}\sum_{\tilde{e} \succ v} s_{v,\tilde{e}}\frac{|\star\tilde{e}|}{|\tilde{e}|}\mathbf{p}_h^\flat(\tilde{e}) \tag{38}$$

where the sign $s_{f,e}$ is +1 if the face $f \succ e$ is in the left of the edge e (-1 otherwise) and $s_{v,e}$ is +1 if the edge $e \succ v$ points to the vertex v and -1 if e points away from v (see figure 1). We see $\mathbf{\Delta}_h^{\mathrm{RR}}$, $\mathbf{\Delta}_h^{\mathrm{GD}}$ and also $\mathbf{\Delta}_h^{\mathrm{dR}} := -\mathbf{\Delta}_h^{\mathrm{RR}} - \mathbf{\Delta}_h^{\mathrm{GD}}$ are linear operators in $\mathbf{p}_h^\flat(\tilde{e})$ and therefor results in sparse matrices if the $\mathbf{p}_h^\flat(\tilde{e})$ are our degree of freedoms.

4.4 Discrete norm

Approximating the norm $\left\|\mathbf{p}^\flat\right\|$ on a edge $e \in \mathcal{E}$ is not so easy like the development of discrete linear operators. We only know how $\mathbf{p}_h^\flat$ "act" on a single edge, so $\mathbf{p}_h^\flat$ gives us only one dimensional informations. In other words, we only know the proportion $\mathbf{p}_h \cdot \mathbf{e} = \mathbf{p}_h^\flat(e)$ of the discrete contravariant vector field $\mathbf{p}_h = \left(\mathbf{p}_h^\flat\right)^\sharp$ in the $\mathbf{e}$ direction, but we don't know the length of $\mathbf{p}_h$ defined on this edge.

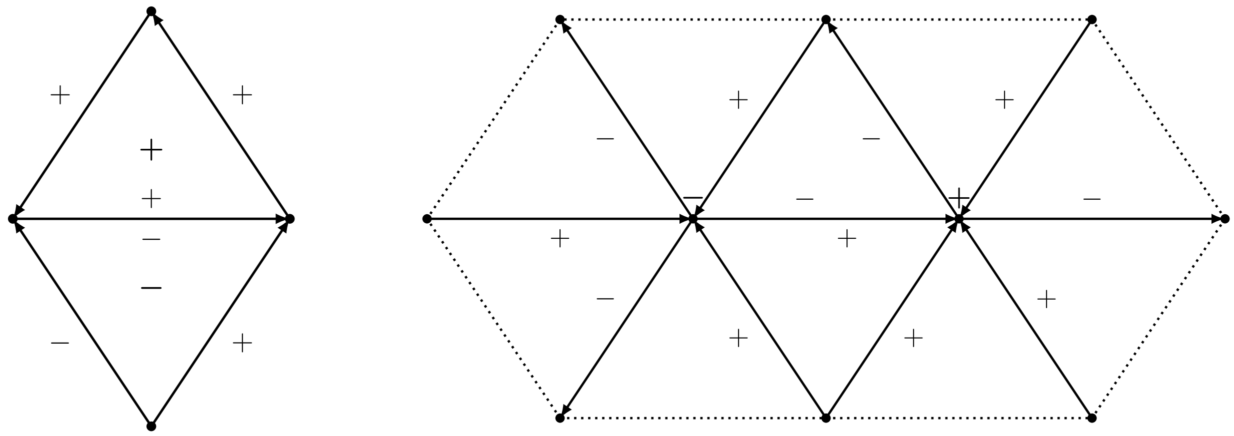

Figure 1: Signs s on example mesh extracts, which affected the discretization of the discrete Laplace operators. Left ($\mathbf{\Delta}_h^{\mathrm{RR}}$): The edge of interest e is the middle edge. The bold signs in the middle of the faces indicate $s_{f,e}$. The other signs at the local edges $\tilde{e}$ (regarding the two faces f) indicate $s_{f,\tilde{e}}$. Right ($\mathbf{\Delta}_h^{\mathrm{GD}}$): The edge of interest e is also the middle edge. The bold signs above the two inner vertices v indicate $s_{v,e}$. The other signs at the local edges $\tilde{e}$ (regarding the two vertices v) indicate $s_{v,\tilde{e}}$.

...maybe some averaging techniques, which I tried and why these sucks...

One way out is to rise the dimension of the discrete 1-forms, therefor we introduce some bases at the intersection $c(e) = e \cap (\star e)$ of a edge and its dual edge to describe discrete contra- and covariant vector fields in a local (piecewise flat) coordinate system.

The basis for contravariant vectors at $c(e)$ is composed of

$$\partial_e X := \mathbf{e} = \mathbf{v}_2 - \mathbf{v}_1 \tag{39}$$

$$\partial_{\star e} X := *\mathbf{e} = c(f_2) - c(f_1) \tag{40}$$

if $e = [v_1, v_2]$ and the face f_1 lay right and f_2 left of e (...figure...). This definitions are consistent with the canonical basis, if the position X is a barycentric parametrisation of the edge e resp. its dual, i.e. for

$$X_e(t_e) = t_e \mathbf{v}_2 + (1 - t_e)\,\mathbf{v}_2 \text{ for } t \in [0, 1] \tag{41}$$

$$X_{\star e}(t_{\star e}) = \begin{cases} 2t_{\star e} c(e) + (1 - 2t_{\star e})\, c(f_1) & \text{if } t_{\star e} \in \left[0, \frac{1}{2}\right] \\ (1 - t_{\star e})\, c(e) + (2t_{\star e} - 1)\, c(f_1) & \text{if } t_{\star e} \in \left[\frac{1}{2}, 1\right] \end{cases} \tag{42}$$

holds $\partial_e X = \partial_{t_e} X_e$ and $\partial_{\star e} X = \frac{1}{2}\left(\partial_{t_{\star e}} X_{\star e}|_{[0,\frac{1}{2}]} + \partial_{t_{\star e}} X_{\star e}|_{[\frac{1}{2},1]}\right)$. Therefore we get the local metric tensor

$$\mathbf{g}_h(e) = |e|^2\,(dx^e)^2 + |\star e|^2\,(dx^{\star e})^2 \tag{43}$$

where $\{dx^e, dx^{\star e}\}$ are the dual base of $\{\partial_e X, \partial_{\star e} X\}$, i.e. $dx^i\,(\partial_j X) = \delta_j^i$ for $i, j \in \{e, \star e\}$. This gives us the great possibility to define

$$\underline{\mathbf{p}}_h^\flat(e) := \mathbf{p}_h^\flat(e) dx^e + \mathbf{p}_h^\flat(\star e) dx^{\star e} = \mathbf{p}_h^\flat(e) dx^e - \frac{|\star e|}{|e|}\left(*\mathbf{p}_h^\flat\right)(e) dx^{\star e} \tag{44}$$

$$= \mathbf{p}_h^\flat(e) \boldsymbol{\xi}^e + \left(*\mathbf{p}_h^\flat\right)(e) \boldsymbol{\xi}^{\star e} =: \begin{bmatrix} \mathbf{p}_h^\flat \\ *\mathbf{p}_h^\flat \end{bmatrix}_{\mathrm{PD}}(e) \tag{45}$$

where $\boldsymbol{\xi}^e := dx^e$ and $\boldsymbol{\xi}^{\star e} := -\frac{|\star e|}{|e|} dx^{\star e}$ are the contravariant Primal-Dual-basis (PD-basis), which we want to use. $\underline{\mathbf{p}}_h^\flat(e)$ is called the discrete Primal-Dual-1-form (PD-1-form). With this scaling and the condition $\boldsymbol{\xi}_i(\boldsymbol{\xi}^j) = \delta_i^j$, it is also possible to define the covariant PD-basis as $\boldsymbol{\xi}_e := \partial_e X$ and $\boldsymbol{\xi}_{\star e} := -\frac{|e|}{|\star e|}\partial_{\star e}X$. Hence, we obtain for the discrete Primal-Dual-vector field (PD-vector field) $\underline{\mathbf{p}}_h$

$$\underline{\mathbf{p}}_h(e) := \left(\underline{\mathbf{p}}_h^\flat(e)\right)^\sharp = \frac{1}{|e|^2}\mathbf{p}_h^\flat(e)\partial_e X + \frac{1}{|\star e|^2}\mathbf{p}_h^\flat(\star e)\partial_{\star e}X \tag{46}$$

$$= \frac{1}{|e|^2}\mathbf{p}_h^\flat(e)\partial_e X - \frac{1}{|e|\,|\star e|}\left(*\mathbf{p}_h^\flat\right)(e)\partial_{\star e}X \tag{47}$$

$$= \frac{1}{|e|^2}\left[\mathbf{p}_h^\flat(e)\boldsymbol{\xi}_e + \left(*\mathbf{p}_h^\flat\right)(e)\boldsymbol{\xi}_{\star e}\right] =: \begin{bmatrix}\mathbf{p}_h^\flat \\ *\mathbf{p}_h^\flat\end{bmatrix}^{\mathrm{PD}}(e) \tag{48}$$

Hence, we get for the square of the norm on $c(e)$ (and also with a constant interpolation on the whole edge) by contract the PD-1-Form with its corresponding PD-Vector

$$\left\|\underline{\mathbf{p}}_h^\flat\right\|_h^2(e) := \left(\underline{\mathbf{p}}_h^\flat\left(\underline{\mathbf{p}}_h\right)\right)(e) = \frac{1}{|e|^2}\left(\left[\mathbf{p}_h^\flat(e)\right]^2 + \left[\left(*\mathbf{p}_h^\flat\right)(e)\right]^2\right) \tag{49}$$

In general, we also get a local discrete inner product between $\underline{\mathbf{p}}_h^\flat$ and another PD-1-form $\underline{\mathbf{q}}_h^\flat$ by

$$\left\langle\underline{\mathbf{q}}_h^\flat, \underline{\mathbf{p}}_h^\flat\right\rangle_h(e) := \left(\underline{\mathbf{q}}_h^\flat\left(\underline{\mathbf{p}}_h\right)\right)(e) = \frac{1}{|e|^2}\left(\left[\mathbf{p}_h^\flat\mathbf{q}_h^\flat\right](e) + \left[\left(*\mathbf{p}_h^\flat\right)\left(*\mathbf{q}_h^\flat\right)\right](e)\right) \tag{50}$$

or a outer product between the PD-1-form $\underline{\mathbf{p}}_h^\flat$ and the PD-vector $\underline{\mathbf{q}}_h$ to produce the PD-(1,1)-Tensor

$$\left(\underline{\mathbf{p}}_h^\flat \otimes \underline{\mathbf{q}}_h\right) := \frac{1}{|e|^2}\left(\mathbf{p}_h^\flat\mathbf{q}_h^\flat\boldsymbol{\xi}^e\otimes\boldsymbol{\xi}_e + \mathbf{p}_h^\flat(*\mathbf{q}_h^\flat)\boldsymbol{\xi}^e\otimes\boldsymbol{\xi}_{\star e} + (*\mathbf{p}_h^\flat)\mathbf{q}_h^\flat\boldsymbol{\xi}^{\star e}\otimes\boldsymbol{\xi}_e + (*\mathbf{p}_h^\flat)(*\mathbf{q}_h^\flat)\boldsymbol{\xi}^{\star e}\otimes\boldsymbol{\xi}_{\star e}\right) \tag{51}$$

$$=: \frac{1}{|e|^2}\begin{bmatrix}\mathbf{p}_h^\flat\mathbf{q}_h^\flat & \mathbf{p}_h^\flat(*\mathbf{q}_h^\flat) \\ (*\mathbf{p}_h^\flat)\mathbf{q}_h^\flat & (*\mathbf{p}_h^\flat)(*\mathbf{q}_h^\flat)\end{bmatrix}_P^D \tag{52}$$

(Arguments (e) are omitted)

5 Discrete PD-Problem, a DEC approach

To use a PD-1-form solution, we must also determine the dual part $*\mathbf{p}_h^\flat$, therefore we discretize the Hodge dual equation (28) (resp. (29)) simultaneous to the primal equation (26) (resp. (27)). This leads to the DEC-discretized Primal-Dual-problem (DEC-PD-problem)

$$\left[\partial_t + K_0\boldsymbol{\Delta}_h^{\mathrm{dR}} + K_n\left(\left\|\underline{\mathbf{p}}_h^\flat\right\|_h^2 - 1\right)\right]\underline{\mathbf{p}}_h^\flat = 0 \tag{53}$$

respective, without the One-Constant-Approximation,

$$\left[\partial_t - \begin{bmatrix}K_1 \\ K_3\end{bmatrix}\boldsymbol{\Delta}_h^{\mathrm{GD}} - \begin{bmatrix}K_3 \\ K_1\end{bmatrix}\boldsymbol{\Delta}_h^{\mathrm{RR}} + K_n\left(\left\|\underline{\mathbf{p}}_h^\flat\right\|_h^2 - 1\right)\right]\underline{\mathbf{p}}_h^\flat = 0 \tag{54}$$

5.1 Time discretization

The simplest way to discretize the DEC-PD-problem in time is to use a implicit Euler scheme, where we handle the norm $\left\|\underline{\mathbf{p}}_h^\flat\right\|_h^2$ explicit. For one Euler step, we have to solve

$$\left[\frac{1}{\tau} + K_0\boldsymbol{\Delta}_h^{\mathrm{dR}} + K_n\left(\left\|\underline{\widehat{\mathbf{p}}}_h^\flat\right\|_h^2(e) - 1\right)\right]\underline{\mathbf{p}}_h^\flat(e) = \frac{1}{\tau}\underline{\widehat{\mathbf{p}}}_h^\flat(e) \tag{55}$$

resp.

$$\left[\frac{1}{\tau} - \begin{bmatrix}K_1 \\ K_3\end{bmatrix}\boldsymbol{\Delta}_h^{\mathrm{GD}} - \begin{bmatrix}K_3 \\ K_1\end{bmatrix}\boldsymbol{\Delta}_h^{\mathrm{RR}} + K_n\left(\left\|\underline{\widehat{\mathbf{p}}}_h^\flat\right\|_h^2(e) - 1\right)\right]\underline{\mathbf{p}}_h^\flat(e) = \frac{1}{\tau}\underline{\widehat{\mathbf{p}}}_h^\flat(e) \tag{56}$$

for all $e \in \mathcal{E}$. $\widehat{\underline{\mathbf{p}}}^\flat_h$ is the solution of the last time step or the initial condition, if this is the first Euler step. $\tau = t - \hat{t}$ is the time step wide.

The drawback of this semi-implicit Euler scheme is, that we need very small τ. Therefore, it is better to use a Taylor-linearisation for $\left\|\underline{\mathbf{p}}^\flat_h\right\|^2_h \underline{\mathbf{p}}^\flat_h$. First we calculate the partially component derivative on a edge $e \in \mathcal{E}$ of

$$\Phi\left(\underline{\mathbf{p}}^\flat_h\right) = \Phi\left(\mathbf{p}^\flat_h, *\mathbf{p}^\flat_h\right) := \left\|\underline{\mathbf{p}}^\flat_h\right\|^2_h \underline{\mathbf{p}}^\flat_h = \frac{1}{|e|^2}\left(\left(\mathbf{p}^\flat_h\right)^2 + \left(*\mathbf{p}^\flat_h\right)^2\right)\begin{bmatrix}\mathbf{p}^\flat_h \\ *\mathbf{p}^\flat_h\end{bmatrix} \tag{57}$$

(Henceforward, for a better readability, the arguments e are omitted). Hence, we obtain

$$\partial_{\mathbf{p}^\flat_h}\Phi = \frac{1}{|e|^2}\begin{bmatrix}3\left(\mathbf{p}^\flat_h\right)^2 + \left(*\mathbf{p}^\flat_h\right)^2 \\ 2\mathbf{p}^\flat_h\left(*\mathbf{p}^\flat_h\right)\end{bmatrix} \tag{58}$$

$$\partial_{*\mathbf{p}^\flat_h}\Phi = \frac{1}{|e|^2}\begin{bmatrix}2\mathbf{p}^\flat_h\left(*\mathbf{p}^\flat_h\right) \\ \left(\mathbf{p}^\flat_h\right)^2 + 3\left(*\mathbf{p}^\flat_h\right)^2\end{bmatrix} \tag{59}$$

For one step Taylor at $\widehat{\underline{\mathbf{p}}}^\flat_h$, we get

$$\begin{aligned}
\Phi(\underline{\mathbf{p}}^\flat_h) &\approx \Phi(\widehat{\underline{\mathbf{p}}}^\flat_h) + \left(\mathbf{p}^\flat_h - \widehat{\mathbf{p}}^\flat_h\right)\partial_{\mathbf{p}^\flat_h}\Phi\left(\widehat{\underline{\mathbf{p}}}^\flat_h\right) + \left(*\mathbf{p}^\flat_h - *\widehat{\mathbf{p}}^\flat_h\right)\partial_{*\mathbf{p}^\flat_h}\Phi\left(\widehat{\underline{\mathbf{p}}}^\flat_h\right) && (60)\\
&= \left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h \widehat{\underline{\mathbf{p}}}^\flat_h + \frac{1}{|e|^2}\begin{bmatrix}\left(\mathbf{p}^\flat_h - \widehat{\mathbf{p}}^\flat_h\right)\left(3\left(\mathbf{p}^\flat_h\right)^2 + \left(*\mathbf{p}^\flat_h\right)^2\right) + 2\left(*\mathbf{p}^\flat_h - *\widehat{\mathbf{p}}^\flat_h\right)\mathbf{p}^\flat_h\left(*\mathbf{p}^\flat_h\right) \\ 2\left(\mathbf{p}^\flat_h - \widehat{\mathbf{p}}^\flat_h\right)\mathbf{p}^\flat_h\left(*\mathbf{p}^\flat_h\right) + \left(*\mathbf{p}^\flat_h - *\widehat{\mathbf{p}}^\flat_h\right)\left(3\left(\mathbf{p}^\flat_h\right)^2 + \left(*\mathbf{p}^\flat_h\right)^2\right)\end{bmatrix} && (61)\\
&= \left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h \widehat{\underline{\mathbf{p}}}^\flat_h - \frac{3}{|e|^2}\left(\left(\widehat{\mathbf{p}}^\flat_h\right)^2 + \left(*\widehat{\mathbf{p}}^\flat_h\right)^2\right)\widehat{\underline{\mathbf{p}}}^\flat_h + \frac{2}{|e|^2}\begin{bmatrix}\left(*\widehat{\mathbf{p}}^\flat_h\right)^2 \\ \left(\widehat{\mathbf{p}}^\flat_h\right)^2\end{bmatrix}\widehat{\underline{\mathbf{p}}}^\flat_h && (62)\\
&\qquad + \frac{1}{|e|^2}\left(\left(\widehat{\mathbf{p}}^\flat_h\right)^2 + \left(*\widehat{\mathbf{p}}^\flat_h\right)^2\right)\underline{\mathbf{p}}^\flat_h + \frac{2}{|e|^2}\begin{bmatrix}\mathbf{p}^\flat_h\widehat{\mathbf{p}}^\flat_h \\ \left(*\mathbf{p}^\flat_h\right)\left(*\widehat{\mathbf{p}}^\flat_h\right)\end{bmatrix}\widehat{\underline{\mathbf{p}}}^\flat_h \\
&\qquad + \frac{2}{|e|^2}\begin{bmatrix}\left(*\mathbf{p}^\flat_h - *\widehat{\mathbf{p}}^\flat_h\right)\left(*\mathbf{p}^\flat_h\right) \\ \left(\mathbf{p}^\flat_h - \widehat{\mathbf{p}}^\flat_h\right)\mathbf{p}^\flat_h\end{bmatrix}\widehat{\underline{\mathbf{p}}}^\flat_h \\
&= -2\left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h \widehat{\underline{\mathbf{p}}}^\flat_h + \left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h \underline{\mathbf{p}}^\flat_h + 2\left\langle \underline{\mathbf{p}}^\flat_h, \widehat{\underline{\mathbf{p}}}^\flat_h\right\rangle_h \widehat{\underline{\mathbf{p}}}^\flat_h && (63)
\end{aligned}$$

The inner product term can be also expressed as matrix-vector multiplication:

$$\left\langle \underline{\mathbf{p}}^\flat_h, \widehat{\underline{\mathbf{p}}}^\flat_h\right\rangle_h \widehat{\underline{\mathbf{p}}}^\flat_h = \frac{1}{|e|^2}\begin{bmatrix}\left(\widehat{\mathbf{p}}^\flat_h\right)^2 & \widehat{\mathbf{p}}^\flat_h\left(*\widehat{\mathbf{p}}^\flat_h\right) \\ \widehat{\mathbf{p}}^\flat_h\left(*\widehat{\mathbf{p}}^\flat_h\right) & \left(*\widehat{\mathbf{p}}^\flat_h\right)^2\end{bmatrix}^D_P \cdot \underline{\mathbf{p}}^\flat_h = \left(\widehat{\underline{\mathbf{p}}}^\flat_h \otimes \widehat{\underline{\mathbf{p}}}_h\right)\cdot \underline{\mathbf{p}}^\flat_h \tag{64}$$

With the Taylor linearization and the implicit Euler scheme, we have to solve the following PD-DEC-Problem in every time steps and all $e \in \mathcal{E}$

$$\left[\frac{1}{\tau} + K_0\mathbf{\Delta}^{\mathrm{dR}}_h + K_n\left(\left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h - 1\right)\right]\underline{\mathbf{p}}^\flat_h + 2K_n\left(\widehat{\underline{\mathbf{p}}}^\flat_h \otimes \widehat{\underline{\mathbf{p}}}_h\right)\cdot\underline{\mathbf{p}}^\flat_h = \left[\frac{1}{\tau} + 2K_n\left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h\right]\widehat{\underline{\mathbf{p}}}^\flat_h \tag{65}$$

resp.

$$\left[\frac{1}{\tau} - \begin{bmatrix}K_1 \\ K_3\end{bmatrix}\mathbf{\Delta}^{\mathrm{GD}}_h - \begin{bmatrix}K_3 \\ K_1\end{bmatrix}\mathbf{\Delta}^{\mathrm{RR}}_h + K_n\left(\left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h - 1\right)\right]\underline{\mathbf{p}}^\flat_h + 2K_n\left(\widehat{\underline{\mathbf{p}}}^\flat_h \otimes \widehat{\underline{\mathbf{p}}}_h\right)\cdot\underline{\mathbf{p}}^\flat_h = \left[\frac{1}{\tau} + 2K_n\left\|\widehat{\underline{\mathbf{p}}}^\flat_h\right\|^2_h\right]\widehat{\underline{\mathbf{p}}}^\flat_h \tag{66}$$

6 Notes on Implementation

6.1 Edge mesh

6.1.1 Iterators

6.2 Matrix assembling

6.3 Sharp and flat interpolations

7 Experiments

7.1 Nonic Surface

We are starting with the standard parametrization ($\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$)

$$X_{\mathbb{S}}(\theta, \phi) = \sin\theta\cos\phi\boldsymbol{\xi}^x + \sin\theta\sin\phi\boldsymbol{\xi}^y + \cos\theta\boldsymbol{\xi}^z \tag{67}$$

of the unit sphere and make a displacement in the $\boldsymbol{\xi}^x$-direction depending on the z-position:

$$X(\theta, \phi) := X_{\mathbb{S}}(\theta, \phi) + f(\cos\theta)\boldsymbol{\xi}^x \tag{68}$$

This results also in an implicit description of this surface in standard Euclidean (x, y, z)-coordinates:

$$\varphi(x, y, z) := (x - f(z))^2 + y^2 + z^2 - 1 = 0 \tag{69}$$

We choose for the displacement function $f : [-1, 1] \to \mathbb{R}$ a double well function, so that the north pole ($z = 1$) of the initial sphere is shifting right in $\boldsymbol{\xi}^x$-direction by $C > 0$ and the south pole ($z = -1$) by $r \cdot C$ with the proportion factor $0 < r < 1$. This implies

$$f_{C,r}(z) = \frac{1}{4}Cz^2\left[(z+1)^2(4-3z) + r(z-1)^2(4+3z)\right] \tag{70}$$

and the double well conditions $f(1) = C$, $f(-1) = rC$ and $f'(1) = f'(0) = f'(-1) = 0$ are fulfilled. We call this subsequent manifold a nonic surface, because the left-hand side of the resulting implicit description (69) is a polynomial of degree 10. The reason why we don't choose $r = 1$ to get a less complex surface is to break the symmetry in the x-y-plane, this is necessary for preventing meta stable states in the dynamic of the orientation fields.

An simple choice for an initial condition is

$$\mathbf{p}_0^\flat = \frac{\mathbf{d}x}{\|\mathbf{d}x\|} \tag{71}$$

because we can discretize $\mathbf{d}x$ on an edge $e = [v_1, v_2]$ by (stokes theorem)

$$(\mathbf{d}x)_h(e) = (v_2 - v_1) \cdot \boldsymbol{\xi}^x = v_2^x - v_1^x \tag{72}$$

independent in the parametrization of the surface. Hence, after normalizing, there are three defects with a positive charge on the three bulges and one defect with a negative charge on the saddle point. (That are the 4 positions, where the tangential space is orthogonal to $\boldsymbol{\xi}^x$.) If needed, by rising the indices we get the surface gradient of the x-component

$$(\mathbf{d}x)^\sharp = \nabla_M x = \left[g_{C,r}^{ij}\partial_j x(\theta, \phi)\right]^{i=\theta,\phi} = \left(I - \frac{\nabla\varphi_{C,r}}{\|\nabla\varphi_{C,r}\|} \otimes \frac{\nabla\varphi_{C,r}}{\|\nabla\varphi_{C,r}\|}\right)\boldsymbol{\xi}^x \tag{73}$$

For the normalizing procedure, it is also the Hodge dual initial solution to discretized (the rotation of the x-component). If the face $f_1 \succ e$ is right of the edge e and $f_2 \succ e$ located left, so that $\star e = [c(f_1), c(f_2)]$ is the dual edge, than we can approximate

$$(*\mathbf{d}x)_h(e) = -\frac{|e|}{|\star e|}(\mathbf{d}x)(\star e) = -\frac{|e|}{|\star e|}\left([c(f_2)]^x - [c(f_1)]^x\right) \tag{74}$$

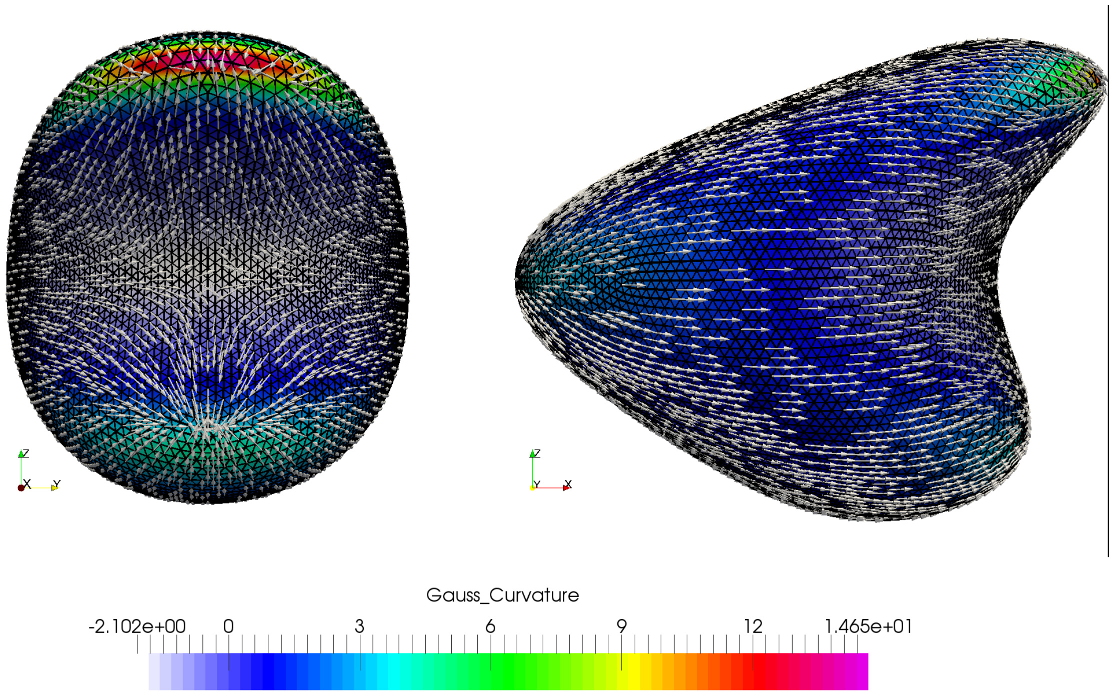

Figure 2: Nonic Surface with shift factor $C = 1$ and proportion factor $r = 0.5$. The mesh is well-centered. The Gauss curvature is plotted too. The arrows show the contravariant initial solution $\mathbf{p}_0$ on some vertices.

With the discrete norm (49) of the PD-1-form, we obtain the initial PD-1-form on $e \in \mathcal{E}$ by

$$\underline{\mathbf{p}}^{\flat}_{h,0}(e) = \frac{\begin{bmatrix} v_2^x - v_1^x \\ -\frac{|e|}{|\star e|}\left([c(f_2)]^x - [c(f_1)]^x\right) \end{bmatrix}_{PD}}{\sqrt{\frac{1}{|e|^2}\left(v_2^x - v_1^x\right)^2 + \frac{1}{|\star e|^2}\left([c(f_2)]^x - [c(f_1)]^x\right)^2}} \tag{75}$$

See figure 2 for the covariant vector field $\mathbf{p}_0$, well centered triangulation and Gauss curvature.

The surface parameters r and C affect the geometric properties and hence the dynamic of the solution behavior and the final equilibrium state. To test the influence of these parameters, we choose a fixed proportion factor $r = 0.99$. This is nearly the symmetric case $r = 1$, but to choose r slightly less than one is to be enough to prevent metastable solutions. By variating of the shift factor $C \in [0.96, 1.00]$ the system rises two fundamental different equilibrium solutions. If $C < 0.98$ then we always get a $\{+, +\}$ charge defect configuration (see figure 3 (bottom)). If $C \geq 0.98$ then the final solution stay a $\{+, +, +, -\}$ configuration (see figure 3 (top)). We choose $K_n = 800$ in the discretized PDE to resolve sufficiently the defect radii. The Frank-Oseen-Energy and the time, when two of the four defects are fusing for $C < 0.98$, are plotted in figure 4.

8 Appendix

8.1 Nonic Surface

References

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[Whi57] H. Whitney. *Geometric Integration Theory*. Princeton mathematical series. University Press, 1957.

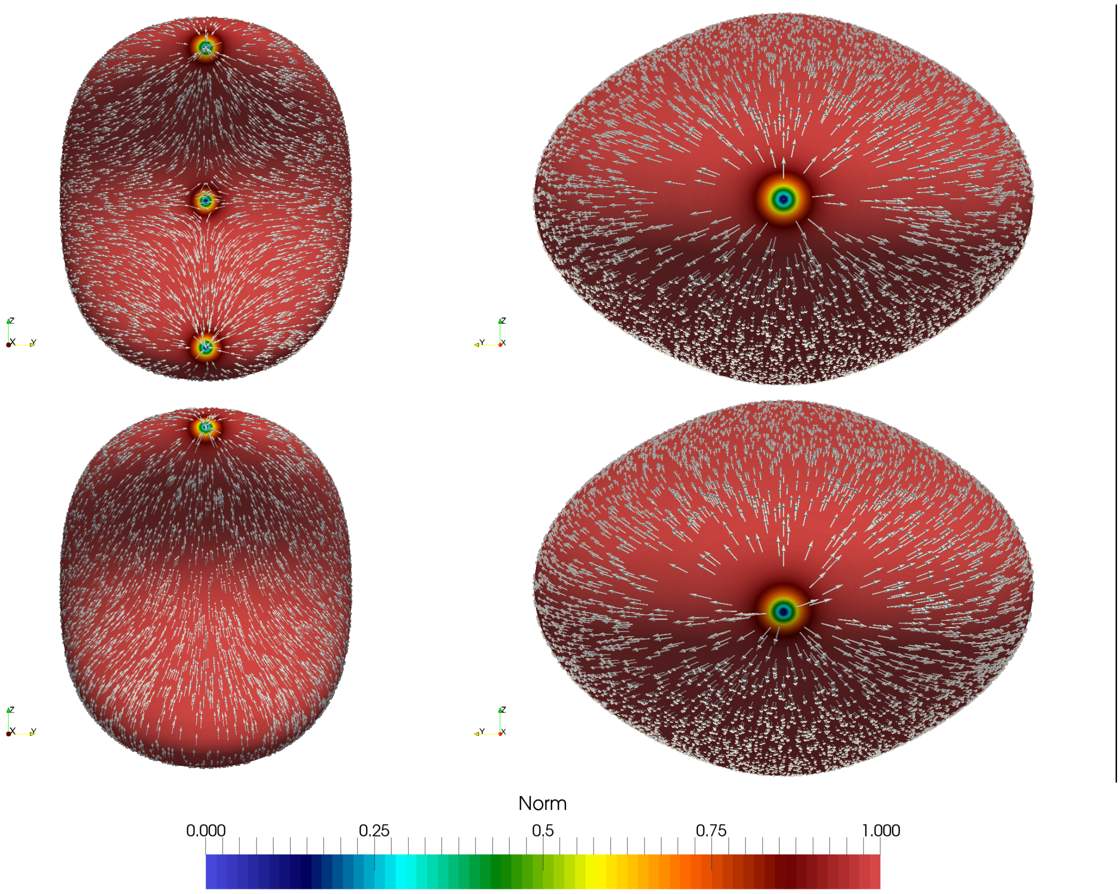

Figure 3: Nonic Surface ($r = 0.99$) with shift factor $C = 1$ (top row) and $C = 0.96$ (bottom row) with view in x-direction (right) and ($-x$)-direction (left). The final contravariant solutions $\mathbf{p}_\infty$ and their norm are plotted for visualising the charge defects. In the top row arises two sinks, one source and one saddle point defects. In the bottom row we get finally only one sink and one source defects, which is slightly below the bulge (right).

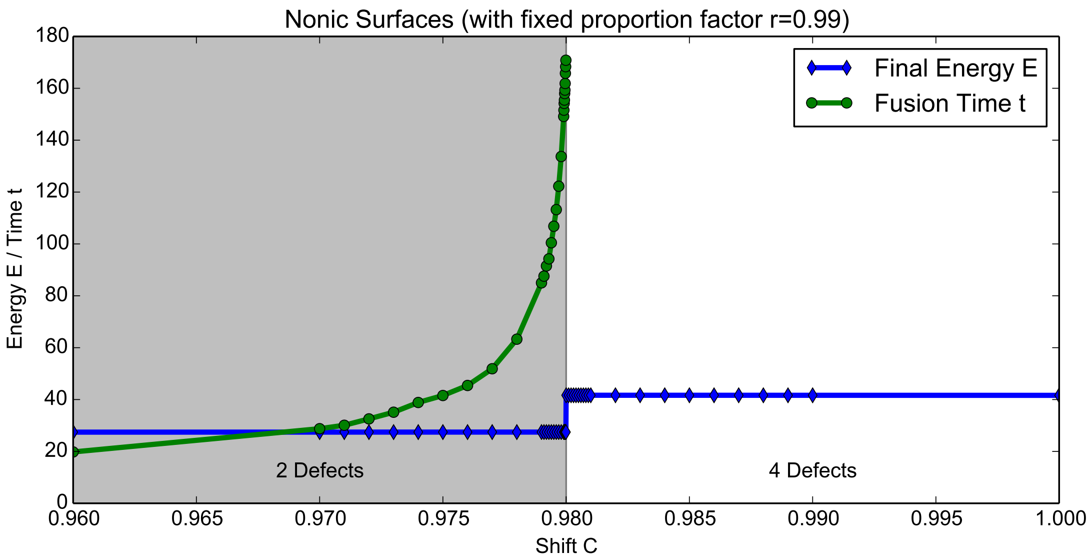

Figure 4: Parameter study for the shift factor $C \in [0.96, 1]$. Plotted are the final Frank-Oseen-Energy and the fusion time, when the shrink defect from the slightly minor bulge and the saddle point defect are fully self-neutralized. This only happens for $C < 0.98$. In the left limes the fusion time becomes singularly. The energy increase only very weakly linear in C up to $C \nearrow 0.98$. After the energy jump (transition from the 2-defects to the 4-defects configuration) the energy decrease also very weakly linear.