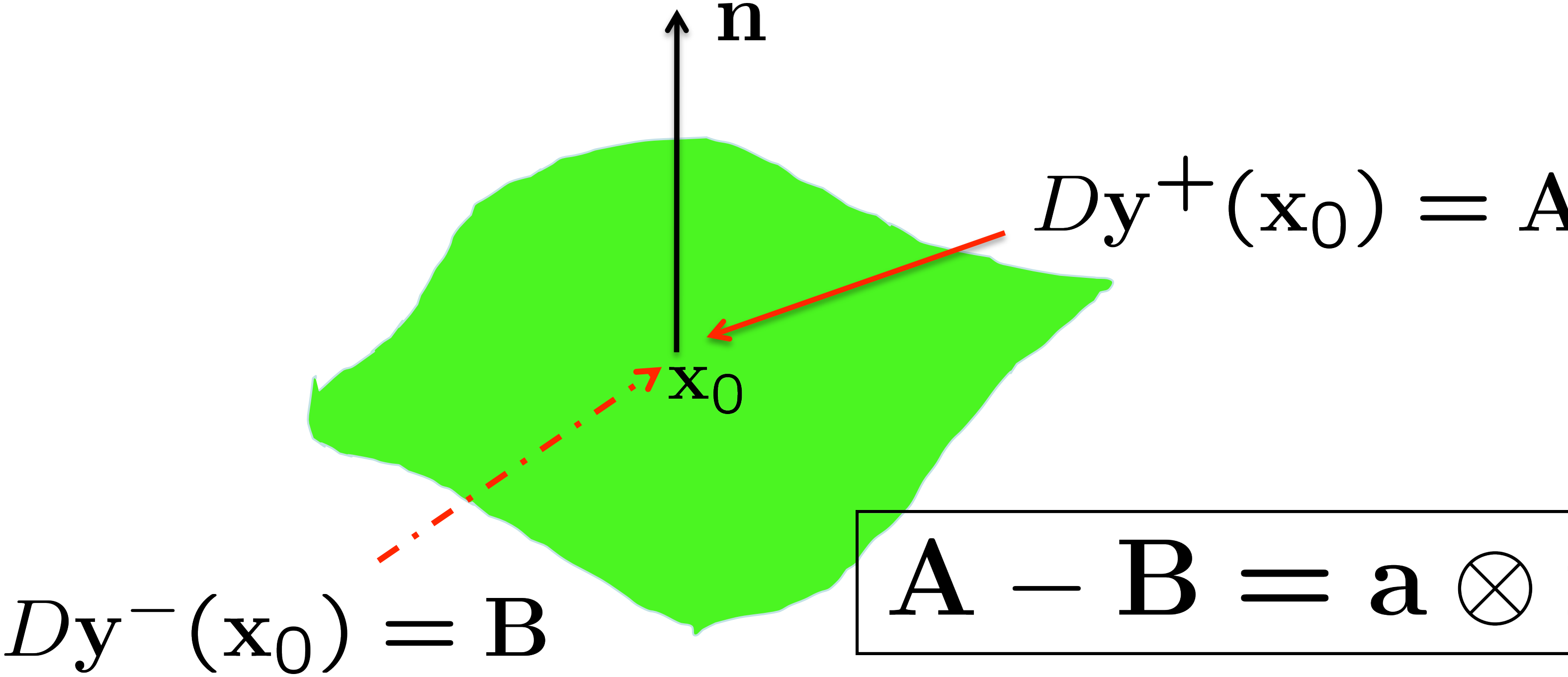
More generally this holds for $\mathbf{y}$ piecewise C^1, with $D\mathbf{y}$ jumping across a C^1 surface.



$$\mathbf{A} - \mathbf{B} = \mathbf{a} \otimes \mathbf{n}$$

(See later for generalizations when $\mathbf{y}$ not piecewise C^1.)

Theorem
Let $\mathbf{U} = \mathbf{U}^T > 0$, $\mathbf{V} = \mathbf{V}^T > 0$. Then $SO(3)\,\mathbf{U}$, $SO(3)\,\mathbf{V}$ are rank-one connected iff

$$\mathbf{U}^2 - \mathbf{V}^2 = c(\mathbf{n} \otimes \tilde{\mathbf{n}} + \tilde{\mathbf{n}} \otimes \mathbf{n}) \qquad (*)$$

for unit vectors $\mathbf{n}$, $\tilde{\mathbf{n}}$ and some $c \neq 0$.
If $\tilde{\mathbf{n}} \neq \pm\mathbf{n}$ there are exactly two rank-one connections between $\mathbf{V}$ and $SO(3)\,\mathbf{U}$ given by

$$\mathbf{R}\mathbf{U} = \mathbf{V} + \mathbf{a} \otimes \mathbf{n}, \quad \tilde{\mathbf{R}}\mathbf{U} = \mathbf{V} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}},$$

for suitable $\mathbf{R}, \tilde{\mathbf{R}} \in SO(3)$, $\mathbf{a}, \tilde{\mathbf{a}} \in \mathbb{R}^3$.

(JB/Carstensen version of standard result cf. Ericksen, Gurtin, JB/James ...)

Proof. Note first that

$$\begin{aligned}\det(\mathbf{V}+\mathbf{a}\otimes\mathbf{n}) &= \det\mathbf{V}\cdot\det(1+\mathbf{V}^{-1}\mathbf{a}\otimes\mathbf{n})\\ &= \det\mathbf{V}\cdot(1+\mathbf{V}^{-1}\mathbf{a}\cdot\mathbf{n}).\end{aligned}$$

Hence if $1+\mathbf{V}^{-1}\mathbf{a}\cdot\mathbf{n}>0$, then by the polar decomposition theorem $\mathbf{RU}=\mathbf{V}+\mathbf{a}\otimes\mathbf{n}$ for some $\mathbf{R}\in SO(3)$ if and only if

$$\begin{aligned}\mathbf{U}^2 &= (\mathbf{V}+\mathbf{n}\otimes\mathbf{a})(\mathbf{V}+\mathbf{a}\otimes\mathbf{n})\\ &= \mathbf{V}^2+\mathbf{Va}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{Va}+|\mathbf{a}|^2\mathbf{n}\otimes\mathbf{n}\\ &= \mathbf{V}^2+\left(\mathbf{Va}+\frac{1}{2}|\mathbf{a}|^2\mathbf{n}\right)\otimes\mathbf{n}+\mathbf{n}\otimes\left(\mathbf{Va}+\frac{1}{2}|\mathbf{a}|^2\mathbf{n}\right).\end{aligned}$$

If $\mathbf{a} \neq \mathbf{0}$ then $\mathbf{Va} + \frac{1}{2}|\mathbf{a}|^2\mathbf{n} \neq \mathbf{0}$, since otherwise

$$\mathbf{Va} \cdot \mathbf{V}^{-1}\mathbf{a} + \frac{1}{2}|\mathbf{a}|^2\mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} = 0,$$

i.e. $2 + \mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} = 0$. This proves the necessity of (*).

Conversely, suppose $(*)$ holds. We need to find $\mathbf{a} \neq \mathbf{0}$ such that $\mathbf{Va} + \frac{1}{2}|\mathbf{a}|^2\mathbf{n} = c\tilde{\mathbf{n}}$ and $1 + \mathbf{V}^{-1}\mathbf{a} \cdot \mathbf{n} > 0$. So we need to find t such that

$$\mathbf{a} = c\mathbf{r} + t\mathbf{s}$$

where $|c\mathbf{r} + t\mathbf{s}|^2 + 2t = 0$ and $1 + (c\mathbf{r} + t\mathbf{s}) \cdot \mathbf{s} > 0$, where we have written $\mathbf{r} = \mathbf{V}^{-1}\tilde{\mathbf{n}}$, $\mathbf{s} = \mathbf{V}^{-1}\mathbf{n}$.

The quadratic for t has the form

$$t^2|\mathbf{s}|^2 + 2t(1 + c\mathbf{r}\cdot\mathbf{s}) + c^2|\mathbf{r}|^2 = 0 \quad \text{with roots}$$

$$t = \frac{-(1 + c\mathbf{r}\cdot\mathbf{s}) \pm \sqrt{(1 + c\mathbf{r}\cdot\mathbf{s})^2 - c^2|\mathbf{r}|^2|\mathbf{s}|^2}}{|\mathbf{s}|^2}.$$

Since $\det \mathbf{U}^2 = \det \mathbf{V}^2 \det(1 + c(\mathbf{r}\otimes\mathbf{s} + \mathbf{s}\otimes\mathbf{r}))$,

$$\det(1 + c(\mathbf{r}\otimes\mathbf{s} + \mathbf{s}\otimes\mathbf{r})) = (1 + c\mathbf{r}\cdot\mathbf{s})^2 - c^2|\mathbf{r}|^2|\mathbf{s}|^2$$

is positive and the roots are real. In order to satisfy $1 + c\mathbf{r}\cdot\mathbf{s} + t|\mathbf{s}|^2 > 0$ we must take the $+$ sign, giving a unique $\mathbf{a}$, and thus unique $\mathbf{R}$ such that $\mathbf{RU} = \mathbf{V} + \mathbf{a}\otimes\mathbf{n}$.

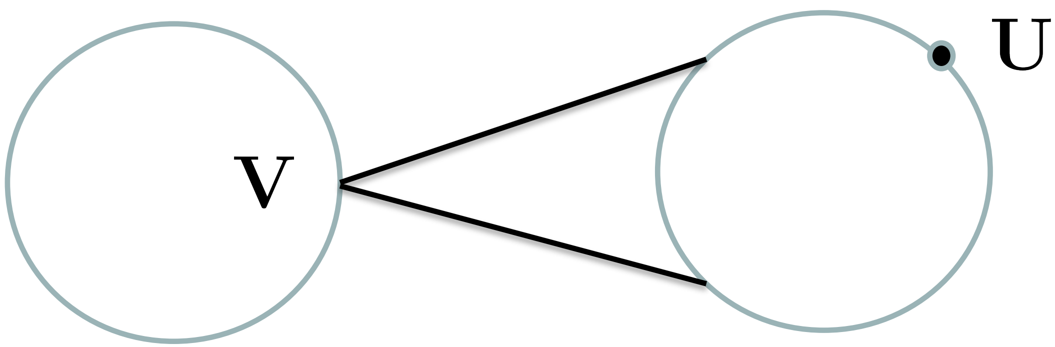
Similarly we get a unique $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{R}}$ such that $\tilde{\mathbf{R}}\mathbf{U} = \mathbf{V} + \tilde{\mathbf{a}} \otimes \tilde{\mathbf{n}}$.

To complete the proof it suffices to check the following

Lemma

If $c(\mathbf{n} \otimes \tilde{\mathbf{n}} + \tilde{\mathbf{n}} \otimes \mathbf{n}) = c'(\tilde{\mathbf{p}} \otimes \mathbf{p} + \mathbf{p} \otimes \tilde{\mathbf{p}})$ for unit vectors $\mathbf{p}, \tilde{\mathbf{p}}$ and some constant c', then either $\mathbf{p} \otimes \tilde{\mathbf{p}} = \pm \mathbf{n} \otimes \tilde{\mathbf{n}}$ or $\mathbf{p} \otimes \tilde{\mathbf{p}} = \pm \tilde{\mathbf{n}} \otimes \mathbf{n}$.

$\square$



Corollaries:

1. There are no rank-one connections between matrices $\mathbf{A}, \mathbf{B}$ belonging to the *same* energy well.

Proof. In this case $\mathbf{U} = \mathbf{V}$, contradicting $c \neq 0$. $\square$

2. There is a rank-one connection between pairs of matrices $\mathbf{A} \in SO(3)$ and $\mathbf{B} \in SO(3)\mathbf{U}$ *if and only if* $\mathbf{U}$ *has middle eigenvalue 1.*

(Thus it is in generically impossible to have an interface between constant gradients in the austenite and martensite energy wells.)

Proof. If there is a rank-one connection then 1 is an eigenvalue since $\det(\mathbf{U}^2 - 1) = 0$.

Choosing $\mathbf{e}$ with $\tilde{\mathbf{n}}\cdot\mathbf{e} > 0, \mathbf{n}\cdot\mathbf{e} > 0$ and $\tilde{\mathbf{n}}\cdot\mathbf{e} > 0$, $\mathbf{n}\cdot\mathbf{e} < 0$, we see that 1 is the middle eigenvalue. Conversely, if

$$\mathbf{U} = \lambda_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda_3 \mathbf{e}_3 \otimes \mathbf{e}_3$$

with eigenvectors $\mathbf{e}_i$ and eigenvalues $\lambda_1 \leq 1 \leq \lambda_3$ then

$$\begin{aligned}\mathbf{U}^2 - \mathbf{1} = \frac{\lambda_3^2 - \lambda_1^2}{2}\Big(&(\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \otimes (-\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \\ &+ (-\alpha\mathbf{e}_1 + \beta\mathbf{e}_3) \otimes (\alpha\mathbf{e}_1 + \beta\mathbf{e}_3)\Big),\end{aligned}$$

where $\alpha = \sqrt{\frac{1-\lambda_1^2}{\lambda_3^2-\lambda_1^2}}, \beta = \sqrt{\frac{\lambda_3^2-1}{\lambda_3^2-\lambda_1^2}}$. $\square$

3. If $\mathbf{U}_i, \mathbf{U}_j$ are distinct martensitic variants then $SO(3)\mathbf{U}_i$ and $SO(3)\mathbf{U}_j$ are rank-one connected if and only if $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$, and the possible interface normals are orthogonal. Variants separated by such interfaces are called *twins*.

Proof. Clearly $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$ is necessary, since the matrix on the RHS of (*) is of rank at most 2.

Conversely suppose that $\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$. Then $\mathbf{U}_i^2 - \mathbf{U}_j^2$ has the spectral decomposition

$$\mathbf{U}_i^2 - \mathbf{U}_j^2 = \lambda \mathbf{e} \otimes \mathbf{e} + \mu \hat{\mathbf{e}} \otimes \hat{\mathbf{e}}.$$

Since $\mathbf{U}_j = \mathbf{R}\mathbf{U}_i\mathbf{R}^T$ for some $\mathbf{R} \in P^{24}$ it follows that $\mathrm{tr}\,(\mathbf{U}_i^2 - \mathbf{U}_j^2) = 0$. Hence $\mu = -\lambda$ and

$$\begin{aligned} \mathbf{U}_i^2 - \mathbf{U}_j^2 &= \lambda(\mathbf{e} \otimes \mathbf{e} - \hat{\mathbf{e}} \otimes \hat{\mathbf{e}}) \\ &= \lambda\left(\frac{\mathbf{e}+\hat{\mathbf{e}}}{\sqrt{2}} \otimes \frac{\mathbf{e}-\hat{\mathbf{e}}}{\sqrt{2}} + \frac{\mathbf{e}-\hat{\mathbf{e}}}{\sqrt{2}} \otimes \frac{\mathbf{e}+\hat{\mathbf{e}}}{\sqrt{2}}\right), \end{aligned}$$

as required. $\square$

Remark: Another equivalent condition due to Forclaz is that $\det(\mathbf{U}_i - \mathbf{U}_j) = 0$. This is because of the surprising identity (not valid in higher dimensions)

$$\det(\mathbf{U}_i^2 - \mathbf{U}_j^2) = (\lambda_1+\lambda_2)(\lambda_2+\lambda_3)(\lambda_3+\lambda_1)\det(\mathbf{U}_i - \mathbf{U}_j).$$