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TIME-DISCRETE INTEGRATION OF FINITE DEFORMATION

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Abstract: *Some necessary implications for the time-discrete integration of finite deformations will be discussed together with particular schemes, when the geometrical structure of the space of Cauchy-Green deformation tensors, implicitly contained in the principle of virtual power, is taken into account. All these time-discrete schemes reflect this geometrical structure in that the actual integration of corresponding evolution equation of deformation process takes place in the subset of positive-definite symmetric matrices (with non-Euclidean geometry), instead of in the linear space of symmetric matrices (with Euclidean geometry) as usual.*

Keywords: ***Finite deformation, time-discrete integration, Runge – Kutta – Munthe-Kaas method.***

1. Introduction

The conference paper is intended to draw attention to one of consequences, namely, the time-discrete approximation of finite deformation, when seeing a deformation process as a curve in the space of deformation tensors – in the sense of Noll and Seguin (2010), though using a rather different mathematical infrastructure and, moreover, employing natural geometry of this space, inherited from the principle of virtual power, see Fiala (2011, 2008). This approach provides exact and geometrically consistent procedure for linearization and integration of deformation process in time variable.

STARTING POINT: From the viewpoint of finite deformations, a deformation process can be represented pointwise by a trajectory $\mathbf{C} : I \to Sym^+(3,\mathbb{R})$ – the configuration space consisting of the set of all positive-definite symmetric matrices (*right Cauchy-Green deformation tensors*).

Note that $\partial\mathbf{C}_t = 2\mathbf{F}^T\mathbf{d}\mathbf{F} \in sym(3,\mathbb{R})$ – the linear vector space of all symmetric matrices, where $\mathbf{d}$ is the *rate-of-deformation* tensor (stretching) – symmetric velocity gradient, and $\mathbf{F}$ is deformation gradient. One can then prove (Fiala (2011, 2008)) the following proposition.

PROPOSITION: Within small deformations, a deformation process superposed on initially strained body, characterized by the initial deformation field $\mathbf{C}$, is represented by a trajectory in the linear vector space of all symmetric matrices $sym(3,\mathbb{R}) \equiv T_{\mathbf{C}}Sym^+(3,\mathbb{R})$ – the tangent space to the manifold $Sym^+(3,\mathbb{R})$ at a point $\mathbf{C}$, i.e. the space of all vectors emanating from $\mathbf{C}$.

Based on the *power of internal forces*, we introduce Riemannian metric on $Sym^+ \equiv Sym^+(3,\mathbb{R})$ to become a manifold with Riemannian geometry, so that we shall be able to analyse deformation process by means of tools of differential geometry. Similarly we set $sym \equiv sym(3,\mathbb{R})$. Let us consider the stress power

$$\frac{\delta E_i}{\delta t} := \int_{\mathcal{S}} (\sigma : d)\, dv = \int_{\mathcal{S}} g^{ik} g^{jl} \sigma_{kl}\, d_{ij}\; dv = \int_{\mathcal{B}} B_t^{ik} B_t^{jl} K_{kl}\, \tfrac{1}{2}\, \partial C_{t\,ij}\, dV = \tag{1}$$

$$= \int_{\mathcal{B}} \mathrm{tr}(\mathbf{B}_t\mathbf{K}_t\mathbf{B}_t(\tfrac{1}{2}\,\partial\mathbf{C}_t))\, dV = \int_{\mathcal{B}} \mathrm{tr}(\mathbf{C}_t^{-1}\mathbf{K}_t\mathbf{C}_t^{-1}(\tfrac{1}{2}\,\partial\mathbf{C}_t))\, dV = \int_{\mathcal{B}} \mathrm{tr}(\mathbf{P}_t(\tfrac{1}{2}\,\partial\mathbf{C}_t))\, dV, \tag{2}$$

where symbol σ, as usual, stands for the Cauchy stress field, $\mathbf{K}_t$ for the *convective stress* and $\mathbf{P}_t = \mathbf{C}_t^{-1}\mathbf{K}_t\mathbf{C}_t^{-1}$ for the *2nd Piola-Kirchhoff stress*.

Now, consulting the analytical mechanics (Marsden et al. (1999)), we can interpret

$$\boldsymbol{\Omega}_{\mathbf{C}}(\,.\,,.\,) := \mathrm{tr}\left(\mathbf{C}^{-1}(.)\mathbf{C}^{-1}(.)\right) \tag{3}$$

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as the Riemannian metric on Sym^+ at the point $\mathbf{C}$ – a particular deformation state, and, as a consequence, the convective stress $\mathbf{K}_t$ as the *vector* and the 2nd Piola-Kirchhoff stress $\mathbf{P}_t$ as the *covector fields* along deformation process $\mathbf{C}_t$. Interestingly – in view of the *logarithmic strain* $\log(\mathbf{C})$, a *geodesic* (i.e. straight line) $\mathbf{C}_t$ connecting two deformation states $\mathbf{C}_1$ and $\mathbf{C}_2$ then reads

$$\mathbf{C}_t = \mathrm{Exp}_{\mathbf{C}_0}(t\mathbf{H}) := \mathbf{C}_0 \exp(t\mathbf{C}_0^{-1}\mathbf{H}), \tag{4}$$

where $\mathbf{H} = \mathbf{C}_0 \log(\mathbf{C}_0^{-1}\mathbf{C}_1)$, and exp, log stands for matrix exponential, resp logarithm.

Now, we can draw conclusions of the geometrical structure of Sym^+ for the *time-discrete integration* of finite deformations. If we calculate, starting from a given deformation state of a body $\mathbf{C}_t$, a deformation increment $\partial\mathbf{C}_t$, based on linearized equations and prescribed increments of external loading and displacement, the new resultant deformation $\mathbf{C}_{t+\Delta t}$ then is obtained by mapping this deformation increment to the space of all deformations Sym^+ starting at the initial state – i.e. by mapping the vector $\partial\mathbf{C}_t$ from the tangent space $T_{\mathbf{C}_t}Sym^+$ at the point $\mathbf{C}_t$ into the space Sym^+. This mapping can be formally expressed in terms of a general formula

$$\mathbf{C}_{t+\Delta t} = \mathrm{Exp}_{\mathbf{C}_t}(\Delta t\, \partial\mathbf{C}_t)\,. \tag{5}$$

In our context of Sym^+, the generalized exponential map (2) adds up an increment of deformation $\mathbf{H} \equiv \partial\mathbf{C}_0 \in T_{\mathbf{C}_0}Sym^+$ to the deformation $\mathbf{C}_0 \in Sym^+$, so that the resulting deformation $\mathbf{C}_1(\mathbf{H}) = \mathrm{Exp}_{\mathbf{C}_0}(\mathbf{H})$ stays in the space of deformations Sym^+. This would not be the case if we just set $\mathbf{C}_1(\mathbf{H}) = \mathbf{C}_0 + \mathbf{H}$ due to neglecting the "shape" of Sym^+ within the linear vector space of symmetric tensors sym.

CONSEQUENCE: Resulting deformation $\mathbf{C}_1(\mathbf{H})$ from adding an increment of deformation $\mathbf{H}$ to the deformation $\mathbf{C}_0$ is given by

$$\mathbf{H} \longmapsto \mathbf{C}_1(\mathbf{H}) \equiv \mathrm{Exp}_{\mathbf{C}_0}(\mathbf{H}) := \mathbf{C}_0 \exp(\mathbf{C}_0^{-1}\,\mathbf{H}) = \tag{6}$$

$$= \mathbf{C}_0 + \mathbf{H} + \tfrac{1}{2!}\,\mathbf{H}\mathbf{C}_0^{-1}\,\mathbf{H} + \tfrac{1}{3!}\,\mathbf{H}\mathbf{C}_0^{-1}\,\mathbf{H}\mathbf{C}_0^{-1}\,\mathbf{H} + \ldots \tag{7}$$

The approach mentioned above is nothing but the forward or explicit Euler's scheme, only conditionally stable, for *evolution equation* of deformation process

$$\partial\mathbf{C}_t = 2\mathbf{C}_t\mathbf{D} \tag{8}$$

evolving on Sym^+, where $\mathbf{D} = \mathbf{F}^{-1}\mathbf{dF}$, which is constant along geodesics.

After having summed up basic facts related to time-discrete integration of finite deformations in this introduction, we shall first discuss the geometry of the underlying configuration space Sym^+ and the properties of evolution equation of finite deformation on this space. Then we introduce methods of its solution in terms of Runge – Kutta – Munthe-Kaas (RKMK), and finely briefly mention another closely related method – again based on Lie group approach.

2. Configuration space Sym^+ – a playing field for finite deformations

Geometry of this space is explained in Fiala (2009), where further references are included. Here, I am going to highlight just some facts, which are substantial for exposition of time-discrete integration. Sym^+ is made up of all possible Cauchy-Green deformation tensors $\mathbf{C}$, in any point X of reference configuration $\mathcal{B}$.

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} \tag{9}$$

As usual, $\mathbf{F}$ denotes deformation gradient of Φ. Cauchy-Green deformation tensors are represented by positive-definite symmetric matrix, and describe local geometry in the vicinity of $x = \Phi(X) \in \mathcal{S}$ in actual configuration from the viewpoint of an observer in reference configuration. In fact, $\mathbf{C}(X)$ in $X \in \mathcal{B}$ is related to an image of metric tensor $\mathbf{g}(x)$ in $x \in \mathcal{S}$ via the deformation Φ.

Since $\mathbf{F} \in GL$ – the group of nonsingular matrices with group operation of matrix multiplication, we have a natural map

$$p : GL \to Sym^+ \qquad \mathbf{F} \mapsto \mathbf{C} := \mathbf{F}^T\mathbf{F}. \tag{10}$$

Let us consider two successive deformations resulting in one single deformation and their deformation gradients

$$\Phi = \Phi_2 \circ \Phi_1 \qquad \mathbf{F} = \mathbf{F}_2\mathbf{F}_1. \tag{11}$$

Then

$$\mathbf{C} = \mathbf{F}_1^T\mathbf{C}_{12}\mathbf{F}_1, \tag{12}$$

where the resulting Cauchy-Green deformation tensors $\mathbf{C}$ is obtained by “translating” by an “amount” $\mathbf{F}_1$ of the Cauchy-Green deformation tensor $\mathbf{C}_{12}$ (standing for the deformation in state 1 with respect state 2). This is nothing but an operation of symmetry on Sym^+ with respect to already introduced metric (3) via group GL:

$$R : GL \times Sym^+ \to Sym^+ \qquad (\mathbf{F},\mathbf{C}) \mapsto \mathbf{F}^T\mathbf{C}\mathbf{F}. \tag{13}$$

This operation is called *right translation*, since $R(\mathbf{F}_2\mathbf{F}_1, .) = R(\mathbf{F}_1, R(\mathbf{F}_2, .))$.

There is also similar approach leading to left translation L related to the Piola deformation tensor $\mathbf{B} = \mathbf{F}\mathbf{F}^T$, for which order of composition of transformations $L(\mathbf{F}_2\mathbf{F}_1, .) = L(\mathbf{F}_2, L(\mathbf{F}_1, .))$, compared to order of matrix multiplication in GL, does not reverse.

Before turning to evolution equation we need yet to specify some properties of Sym^+. Since many elements of GL have the same image in Sym^+, the map (10) does not have an inverse. But taking into account polar decomposition of nonsingular matrices $\mathbf{F} = \mathbf{R}\mathbf{U}$, we can introduce the isotropy subgroup $O \subset GL$, which is the group of orthogonal matrices

$$O := \left\{\mathbf{R} \in GL \,|\, \mathbf{R}^T\mathbf{R} = \mathbf{I}\right\}, \tag{14}$$

so that all elements in the *right coset* $[\mathbf{U}] := \{\mathbf{R}\mathbf{U} \,|\, \mathbf{R} \in O\}$ will have the same image $\mathbf{U}^2 \in Sym^+$, and resulting in factorisation of GL into disjoint right cosets. The correspondence between right coset space GL/O and Sym^+

$$\pi : GL/O \to Sym^+ \qquad [\mathbf{F}] \mapsto \mathbf{C} := \mathbf{G}^T\mathbf{G} \quad \text{for some } \mathbf{G} \in [\mathbf{F}] \tag{15}$$

is now one-to-one, and in addition to that, it is diffeomorphism.

Moreover, we can carry over the operation of matrix multiplication in GL to operation of right translations on GL/O via

$$\rho : GL \times GL/O \to GL/O \qquad (\mathbf{G}, [\mathbf{F}]) \mapsto [\mathbf{F}\mathbf{G}], \tag{16}$$

so that the folowing diagram is commutative

$$\begin{tikzcd} GL/O \arrow[r, "\pi"] & Sym^+ \\ GL/O \arrow[r, "\pi"] \arrow[u, "\rho_{\mathbf{G}}"] & Sym^+ \arrow[u, "R_{\mathbf{G}}"'] \end{tikzcd}$$

That is

$$\pi \circ \rho_{\mathbf{G}} = R_{\mathbf{G}} \circ \pi, \tag{17}$$

where $\rho_{\mathbf{G}}(.) := \rho(\mathbf{G}, .)$ and $R_{\mathbf{G}}(.) := R(\mathbf{G}, .)$ for any $\mathbf{G} \in GL$. We call this property *equivariance*, which means that instead of studying the action of GL on Sym^+, we can equally well study the action of GL on GL/O.

3. Evolution equation for finite deformations

After having computed an increment of deformation $\mathbf{d}(v) = sym(\nabla v)$ superposed on a deformed configuration Φ_1 with deformation gradient $\mathbf{F}_1$ and deformation tensor $\mathbf{C}_1$, we have then to update deformation tensor to get the resulting $\mathbf{C}_2$ in terms of the initial $\mathbf{C}_1$ and computed deformation rate

$\partial\mathbf{C}_1 = 2\mathbf{F}_1^T\mathbf{d}(v)\mathbf{F}_1$. Since $\mathbf{F}^T\mathbf{d}\mathbf{F} = \mathbf{C}_t\mathbf{F}^{-1}\mathbf{d}\mathbf{F} = \mathbf{C}_t\mathbf{D}$, see Fiala (2008), we thus obtain the *evolution equation* for deformation process in finite deformations

$$\partial\mathbf{C}_t = 2\mathbf{C}_t\mathbf{D}\left(= 2\mathbf{D}^T\mathbf{C}_t\right) \in T_{\mathbf{C}_t}Sym^+, \tag{18}$$

evolving on $Sym^+ \subset sym$. Its time-discrete integration then gives us the desired formulae for updating deformation tensors $\mathbf{C}_t$. Note that $\mathbf{D} = \mathbf{F}^{-1}\mathbf{d}\mathbf{F}$ is constant along geodesics.

If the equation (18) evolved on the space of symmetric tensors sym, which is linear vector space, we could use Runge – Kutta method, but not in our case of $Sym^+ \subset sym$. In fact, the curve $\mathbf{C}_t$ lies in Sym^+, and so $\partial\mathbf{C}_t \in T_{\mathbf{C}_t}Sym^+$ is the tangent to this curve, i.e. a vector in Sym^+ at its initial point $\mathbf{C}_t$. Since Sym^+ has non-Euclidean geometry, we cannot identify the space of points with the space of all vectors emanating from a point, as is the case for linear vector spaces (with Euclidean geometry), and so the classical Runge – Kutta method is inapplicable. Nevertheless, due to correspondence between the right coset space GL/O and Sym^+, and specific properties of Lie groups GL and O, it is still possible to extend this approach into modified Runge – Kutta – Munthe-Kaas method, which is now usable in our space. The key point is that these spaces possess *"sufficient" amount of "basic" movements*, so that we can still compare different vector spaces at different points, though with a bit complicated formulae in comparison with linear vector spaces (cf. section 5.), for which they simply reduces to identities.

In general, consider a differential equation of the form

$$\partial\mathbf{C} = \mathbf{H}(\mathbf{C}), \qquad t \geq 0, \qquad \mathbf{C}(0) = \mathbf{C}_0, \tag{19}$$

where $\mathbf{H}(\mathbf{C})$ is a tangent vector field on Sym^+. Whenever convenient, we allow $\mathbf{H}$ to be a function of time $\mathbf{H} = \mathbf{H}(t, \mathbf{C})$. The *flow* of a vector field $\mathbf{H}$ is the solution operator

$$\Psi_{t,\mathbf{H}} : Sym^+ \to Sym^+, \tag{20}$$

such that

$$\mathbf{C}(t) = \Psi_{t,\mathbf{H}}(\mathbf{C}_0) \tag{21}$$

solves (19). Note that the vector field $\mathbf{H}$ and the solution operator $\Psi_{t,\mathbf{H}}$ are related by differentiation

$$\mathbf{H}(\mathbf{C}_t) = \left.\frac{d}{dt}\Psi_{t,\mathbf{H}}(\mathbf{C}_t)\right|_{t=0}. \tag{22}$$

Let us now discuss the right-hand side of equation (18) from the viewpoint of basic movements. It is a simple task to prove that

$$\begin{aligned} \partial\mathbf{C}_t &= \mathbf{D}^T\mathbf{C}_t + \mathbf{C}_t\mathbf{D} && (23)\\ &= \mathbf{U}_t\left(\mathbf{R}^{-1}\mathbf{d}\mathbf{R}\right)\mathbf{U}_t, && (24) \end{aligned}$$

where $\mathbf{F}_t = \mathbf{R}_t\mathbf{U}_t$ and $\mathbf{U}_t^2 = \mathbf{C}_t$.

Now, denoting by $R^{\mathbf{C}_0} := R(., \mathbf{C}_0)$, i.e.

$$R^{\mathbf{C}_0} : GL \to Sym^+ \qquad \mathbf{F} \mapsto \mathbf{F}^T\mathbf{C}_0\mathbf{F}, \tag{25}$$

and by $Q^{\mathbf{U}_0}$

$$Q^{\mathbf{U}_0} : Sym^+ \to Sym^+ \qquad \mathbf{B} \mapsto \mathbf{U}_0\mathbf{B}\mathbf{U}_0, \tag{26}$$

then evidently

$$R^{\mathbf{C}_0}(\mathbf{I}) = \mathbf{C}_0 \tag{27}$$

$$Q^{\mathbf{U}_0}(\mathbf{I}) = \mathbf{U}_0^2 = \mathbf{C}_0, \tag{28}$$

and the corresponding vector spaces at $\mathbf{I}$ for both GL and Sym^+ transforms into $T_{\mathbf{C}_0}Sym^+$ by

$$R_*^{\mathbf{C}_0} \equiv T_{\mathbf{I}}R^{\mathbf{C}_0} : T_{\mathbf{I}}GL \to T_{\mathbf{C}_0}Sym^+ \qquad \mathbf{D} \mapsto \mathbf{D}^T\mathbf{C}_0 + \mathbf{C}_0\mathbf{D} \tag{29}$$

$$Q_*^{\mathbf{U}_0} \equiv T_{\mathbf{I}}Q^{\mathbf{U}_0} : T_{\mathbf{I}}Sym^+ \to T_{\mathbf{C}_0}Sym^+ \qquad \hat{\mathbf{D}} \mapsto \mathbf{U}_0\hat{\mathbf{D}}\mathbf{U}_0. \tag{30}$$

Remind that $T_{\mathbf{C}}Sym^+$ is a vector space of all vectors emanating from a point $\mathbf{C} \in Sym^+$, and similarly for the vector space $T_{\mathbf{G}}GL$.

That is,

$$\mathbf{D} = \mathbf{F}^{-1}\mathbf{dF} \in T_{\mathbf{I}}GL \tag{31}$$

$$\hat{\mathbf{D}} = \mathbf{R}^{-1}\mathbf{dR} \in T_{\mathbf{I}}Sym^+ \tag{32}$$

and equation (18) reads

$$\partial\mathbf{C}_t = R_*^{\mathbf{C}_t}(\mathbf{D}_t) \equiv R_*(\mathbf{D}_t)(\mathbf{C}_t) \tag{33}$$

$$= Q_*^{\mathbf{U}_t}(\hat{\mathbf{D}}_t) \equiv Q_*(\hat{\mathbf{D}}_t)(\mathbf{C}_t)\,, \tag{34}$$

where now $\mathbf{D}_t$ is a curve in the vector space of all matrices $\mathfrak{gl} := T_{\mathbf{I}}GL$, and $\hat{\mathbf{D}}_t$ a curve in the vector space of all symmetric matrices $sym := T_{\mathbf{I}}Sym^+$. These equations are called **equations of Lie type** (Munthe-Kaas (1999); Iserles et al. (2000)).

Actually, we made use of an identification $TGL \approx GL \times \mathfrak{gl}$ and $TSym^+ \approx TSym^+ \times sym$, called the *right trivialization*, where $TSym^+$ stands for a disjunct union of all vector spaces $T_{\mathbf{C}}Sym^+$ indexed by $\mathbf{C} \in Sym^+$ and similarly for TGL. Note also that $\mathfrak{gl} := T_{\mathbf{I}}GL = sym \oplus skew$, that is $T_{[\mathbf{I}]}GL/O \equiv sym$ and $T_{\mathbf{I}}O = skew$, see Fiala (2009) and references therein. Notation $skew$ stands for the vector space of all skew-symmetric matrices.

4. Limitations of Runge – Kutta method

The classical ν-stage Runge – Kutta method (Hairer et al. (1993)) is defined by constants $\{a_{k,l}\}_{k,l=1}^{\nu}$, $\{b_l\}_{l=1}^{\nu}$ and $\{c_k\}_{k=1}^{\nu}$, usually written as a *Butcher tableau*

$$\begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \dots & a_{1,\nu} \\ c_2 & a_{2,1} & a_{2,2} & \dots & a_{2,\nu} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_\nu & a_{\nu,1} & a_{\nu,2} & \dots & a_{\nu,\nu} \\ \hline & b_1 & b_2 & \dots & b_\nu \end{array} \tag{35}$$

Applied to a standard vector equation $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ on $\mathbb{R}^n$, a single step of length h from $\boldsymbol{y}_n = \boldsymbol{y}(t_n)$ to updated $\boldsymbol{y}_{n+1} = \boldsymbol{y}(t_n + h)$ is given first by solving following system of equations for $\boldsymbol{f}_l$

$$\left.\begin{array}{l} \boldsymbol{f}_k = \boldsymbol{f}(t_n + c_k h, \boldsymbol{y}_n + h\boldsymbol{\theta}_k) \\ \text{where } \boldsymbol{\theta}_k = \sum_{l=0}^{\nu} a_{k,l}\boldsymbol{f}_l \end{array}\right\} \qquad k = 1, \dots, \nu \tag{36}$$

and then followed by

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\boldsymbol{\theta}, \quad \text{where } \boldsymbol{\theta} = \sum_{l=0}^{\nu} b_l \boldsymbol{f}_l\,. \tag{37}$$

That is, the Runge – Kutta method starts by calculating the the rate of change $\boldsymbol{\theta}$ as a weighted average of estimates of the rate of change of $\boldsymbol{y}$ at several points $t_n + c_k h$ within the interval t_n to t_{n+1}.

Notice that $\boldsymbol{y}$ is a point whereas $\boldsymbol{f}(t, \boldsymbol{y})$ a vector at $\boldsymbol{y}$, which can be translated to the origin of coordinates without a change. In fact, $\mathbb{R}^n$ plays a triple role here: the space of points, then the additive group of translation operating on the space of point, and finally the vector space, on which the actual integration is carried out.

In our case, the space of points is the space Sym^+ made up of all Cauchy-Green deformation tensors, and the transformation group GL stands for the group of translation. Since Runge – Kutta method (RK) demands for $\mathbb{R}^n$, we have to resort to a related linear vector space, which is naturally isomorphic to $\mathbb{R}^n$, provided we properly transform all the quantities and desired operation to this vector space and back to Sym^+. The previous section suggests two of them: either the tangent space $T_{\mathbf{I}}Sym^+$ at the identity matrix $\mathbf{I}$, being equal to the space of all tangents to deformation processes passing through undeformed state – the vector space of all symmetric matrices sym, or $T_{\mathbf{I}}GL$ identified with the vector space of all matrices $\mathfrak{gl}$.

5. Runge – Kutta – Munthe-Kaas method (RKMK)

Following Munthe-Kaas (1999), we point out the role of actions (25) and (26) for constructing modified RK method on general homogeneous spaces: First, instead of seeking the discretization directly on a homogeneous space, we find an element of the group whose action induces the approximation. In fact, in (33) and (34) we expressed evolving equation (19) in the form

$$\partial \mathbf{C}_t = \mathbf{\Lambda}_*(\mathbf{\Delta}_t)(\mathbf{C}_t), \qquad t \geq 0, \qquad \mathbf{C}(0) = \mathbf{C}_0, \tag{38}$$

where either $\mathbf{\Lambda}_* : \mathfrak{gl} \times Sym^+ \to TSym^+$ with a curve $\mathbf{\Delta}_t = \mathbf{D}_t \subset \mathfrak{gl}$, or $\mathbf{\Lambda}_* : sym \times Sym^+ \to TSym^+$ with $\mathbf{\Delta}_t = \hat{\mathbf{D}}_t \subset sym$. In case of time-independent $\mathbf{\Delta}$, the solution of (38), and thus of (19), is given explicitly (Theorem 2.8, Iserles et al. (2000)) in terms of the actions (25) or (26)

$$\mathbf{C}(t) = \mathbf{\Lambda}(\mathbf{\Gamma}_t, \mathbf{C}_0), \quad t \geq 0, \quad \mathbf{\Gamma}_0 = \mathbf{I}, \tag{39}$$

where

$$\mathbf{\Gamma}_t = \text{EXP}(t\Delta_0), \quad \text{i.e.} \quad \partial \mathbf{\Gamma}_0 = \mathbf{\Delta}_0. \tag{40}$$

EXP stands for the matrix exponential. Otherwise, (39) approximates the solution for short times. Equation for Γ_t on corresponding spaces then reads

$$\partial \mathbf{\Lambda}(\mathbf{\Gamma}_t, \mathbf{C}_0) = \mathbf{\Lambda}_*(\mathbf{\Delta}_t)(\mathbf{C}_t), \quad t \geq 0, \quad \mathbf{\Gamma}_0 = \mathbf{I}. \tag{41}$$

That is, instead of approximating $\mathbf{C}(t)$, we seek an approximate action $\mathbf{\Gamma}_t$ that carries $\mathbf{C}(0)$ to $\mathbf{C}(t)$. Moreover, even though the group GL, resp the space Sym^+ are nonlinear objects, it is possible to transform the problem to their related linear spaces $\mathfrak{gl} = T_{\mathbf{I}}GL$, resp $sym = T_{\mathbf{I}}Sym^+$. In these spaces we can already apply calssical RK method and so, after transformating back, we get desired numerical approximation. Coming to terms with all the subtleties results in RKMK method presented in section 5. Notice that the first approach relies on group action GL, whereas the second one makes use of a direct map between the homogeneous space Sym^+ and the linear vector space sym.

As for EXP, let us remind relation of the spaces Sym^+ and GL with their tangent spaces sym and $\mathfrak{gl}$. For more see, for example, Marsden et al. (1999). Denote by $\exp$ and $\mathfrak{exp}$ the usual matrix exponential, but related to different spaces. Whereas $\exp$ maps all sym onto all Sym^+ in one-to-one way, for GL this property does not apply completely. Still, the map $\mathfrak{exp} : \mathfrak{gl} \to GL$ is one-to-one in some vicinity of $\mathfrak{gl}$ at the null matrix $\mathbf{0}$, which is maped onto near vicinity of GL of the identity matrix $\mathbf{I}$, see Fiala (2009). That is, only for those $\mathbf{G} \in GL$ sufficiently close to $\mathbf{I} = \mathfrak{exp}(\mathbf{0})$, there exists precisely one $\mathbf{g} \in \mathfrak{gl}$, such that $\mathbf{G} = \mathfrak{exp}(\mathbf{g})$, with its line segment $\mathfrak{exp}(t\mathbf{g})$ completely lying in this vicinity for $|\,t| \leq 1$. In other word, for any $\mathbf{g} \in \mathfrak{gl}$, one can still find sufficiently small $\varepsilon > 0$, such that a line segment $\mathfrak{exp}(t\mathbf{g})$ is all in this vicinity for $|\,t| \leq \varepsilon$.

During an analysis of the evolution equation for finite deformations, we naturally established two linear vector spaces, namely $sym \equiv T_{\mathbf{I}}Sym^+$ and $\mathfrak{gl} \equiv T_{\mathbf{I}}GL$. In appendix, a transformation of deformation rate fields on Sym^+ and corresponding vector fields on these linear vector spaces is briefly summarized, so that we can now express the evolution equation here.

The equation on linear vector space (sym or $\mathfrak{gl}$) for sufficiently small t reads (see Appendix)

$$\partial \mathbf{\Theta}_t = \text{dEXP}^{-1}_{\mathbf{\Theta}_t}(\mathbf{\Delta}_t)(\mathbf{C}_t), \quad t \geq 0, \quad \mathbf{\Theta}_0 = \mathbf{0}. \tag{42}$$

Now, we can apply RK method to obtain ν-stage Runge – Kutta – Munthe-Kaas method (Munthe-Kaas (1999)) solving our equation $\partial \mathbf{C}_t = \mathbf{\Lambda}_*(\mathbf{\Delta}_t)(\mathbf{C}_t)$, which evolves on Sym^+. Using the *Butcher tableau* (35), one step of RKMK method consists in solving following system of equations for δ_l

$$\left.\begin{aligned} &\mathbf{\Delta}_k = \mathbf{\Delta}\big(t_n + c_k h, \mathbf{\Lambda}\big(\text{EXP}(h\mathbf{\Theta}_k), \mathbf{C}_n\big)\big) \\ &\text{where } \mathbf{\Theta}_k = \textstyle\sum_{l=0}^{\nu} a_{k,l}\delta_l \\ &\qquad \delta_l = \text{dEXP}^{-1}_{\mathbf{\Theta}_l}(\mathbf{\Delta}_l) \end{aligned}\right\} \qquad k = 1, \ldots, \nu \tag{43}$$

then followed by an update

$$\mathbf{C}_{n+1} = \mathbf{\Lambda}\big(\mathrm{EXP}(h\mathbf{\Theta}), \mathbf{C}_n\big), \qquad \text{where } \mathbf{\Theta} = \sum_{l=0}^{\nu} b_l \delta_l \,. \tag{44}$$

Again, $\mathbf{\Lambda}$ stands for the actions (25) or (26), EXP and $\mathbf{d}\mathrm{EXP}^{-1}$ for their corresponding matrix exponentials and their inverse differentials.

In particular:

- forward Euler ($\nu = 1$), cf. (5)

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad\qquad \mathbf{\Theta} = \mathbf{\Delta}(t_n, \mathbf{C}_n) \tag{45}$$

- trapezoidal = modified Euler ($\nu = 2$), for example

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{aligned} \delta_1 &= \mathbf{\Delta}(t_n, \mathbf{C}_n) \\ \delta_2 &= \mathbf{\Delta}\big(t_n + h, \Lambda\big(\mathrm{EXP}(\tfrac{1}{2}\, h(\delta_1 + \delta_2), \mathbf{C}_n)\big)\big) \\ \mathbf{\Theta} &= \tfrac{1}{2}\,(\delta_1 + \delta_2) \end{aligned} \tag{46}$$

6. Conclusions

We analysed the evolution equation for finite deformations. We proved that instead of considering it on the linear vector space of symmetric matrices sym, it actually evolves on its subset – the manifold of symmetric positive definite matrices $Sym^+ \subset sym$, so that the usual time-discrete integration schemes are inapplicable. However, thanks to the specific geometry of Sym^+, due to the principle of virtual power, the modified RK method, namely the Runge – Kutta – Munthe-Kaas method applies. Moreover, the closely related Magnus expansion method, based on the same geometric approach, might prove especially useful for highly-oscillatory problems, see Iserles et al. (2000).

Appendix

To find out the evolution equation on linear vector space, we have yet to work out how to transform deformation rates. For details, see Engø (2000), for preliminaries, for example Marsden et al. (1999). This section is rather technical and is meant only as a reference.

In $T\exp$, the symbol T denotes the tangent lift of a map $\exp$ between manifolds to a map between corresponding tangent bundles (manifolds of vectors) $Tsym$ and $TSym^+$. Since for vector space sym in general $Tsym \approx sym \times sym$, and for Sym^+ in particular $TSym^+ \approx Sym^+ \times T_{\mathbf{I}}Sym^+ \equiv Sym^+ \times sym$, a vector space $T_{\mathbf{\Theta}}sym$ at $\mathbf{\Theta} \in sym$ can be directly identified with sym and a vector space $T_{\mathbf{C}}Sym^+$ at $\mathbf{C}$ with sym through the translation $Q^{\mathbf{U}}$ by $\mathbf{U}$, for which $\mathbf{C} = \mathbf{U}^2$. That is

$$\begin{tikzcd} sym \arrow[r, "id"] & Tsym \arrow[r, "T\exp"] & TSym^+ \arrow[r, "(Q^{\mathbf{U}})^*"] & sym \\ sym \arrow[r, "id"] \arrow[u, "\partial\mathbf{\Theta}"] & sym \arrow[r, "\exp"] \arrow[u, "\partial\mathbf{\Theta}"] & Sym^+ \arrow[r, "Id"] \arrow[u, "\partial\mathbf{C}"'] & Sym^+ \arrow[u, "\mathbf{\Delta}"'] \end{tikzcd}$$

where $(Q_{\mathbf{U}})^* = (Q_{\mathbf{U}})_*^{-1}$. Id and id are respective identity mappings, and in the upper rightmost corner, we made use of the equivalence $T_{\mathbf{I}}Sym^+ \approx sym$. Due to commutativity of the diagram, we eventually conclude

$$\partial\mathbf{\Theta} = \mathbf{d}\exp_{\mathbf{\Theta}}^{-1}\big(\mathbf{\Delta}\big)(\mathbf{C}), \qquad \mathbf{C} = \exp\mathbf{\Theta} \tag{47}$$

where $\partial\mathbf{\Theta}$ is a vector field on sym, and $\mathbf{\Delta}$ a vector field on Sym^+ in right trivialization. Both fields correspond to $\partial\mathbf{C}$ – the deformation rate field on Sym^+. The diagram for $\mathfrak{gl}$ and GL looks similar, see Engø (2000).

Finally, we cite expressions for the inverse of differential of the exponential mapping **d**EXP (inverse of the right-trivialized tangent of the exponential map *T*EXP).

First consider case of $\exp : sym \to Sym^+$. Let now $\boldsymbol{\Theta} = \mathbf{R}\boldsymbol{\Lambda}\mathbf{R}^{\mathrm{T}} = \sum \lambda_i P_i$ be the spectral decomposition of $\boldsymbol{\Theta}$, where $\boldsymbol{\Lambda}$ is the corresponding diagonal matrix with diagonal entries λ_i and P_i corresponding projectors, then (Bhatia (2007))

$$\mathbf{d}\exp_{\boldsymbol{\Theta}}^{-1}(\boldsymbol{\Delta}) := \mathbf{R}\left[\log^{[1]}(\boldsymbol{\Lambda}) \circ (\mathbf{R}^{\mathrm{T}}\boldsymbol{\Delta}\mathbf{R})\right]\mathbf{R}^{\mathrm{T}} \tag{48}$$

$$= \sum_i \sum_j \log^{[1]}(\lambda_i, \lambda_j) P_i \,\boldsymbol{\Delta} P_j, \tag{49}$$

where the *Hadamard (or Schur) product* $\mathbf{A} \circ \mathbf{B}$ of two matrices $\mathbf{A}$ and $\mathbf{B}$ is defined to be the matrix whose (i, j)-entry is $A_i^j B_i^j$, and the 3×3 symmetric matrix $\log^{[1]}(\boldsymbol{\Lambda})$ has numbers

$$\log^{[1]}(\lambda_i, \lambda_j) = \frac{\log(\lambda_i) - \log(\lambda_j)}{\lambda_i - \lambda_j} \quad \text{if } i \neq j \tag{50}$$

$$\log^{[1]}(\lambda_i, \lambda_i) = \log{}'(\lambda_i) = \frac{1}{\lambda_i} \tag{51}$$

as its (i, j)-entries. At point $\mathbf{0} \in sym$ the mapping $\mathbf{d}\exp_{\mathbf{0}}^{-1} = \mathbf{I}$.

Second, making use of the relation $\mathfrak{exp} : \mathfrak{gl} \to GL$ between vector space $\mathfrak{gl}$ and the original space GL results in following relations. Denoting by $[\boldsymbol{\Theta}, \boldsymbol{\Delta}] := \boldsymbol{\Theta}\boldsymbol{\Delta} - \boldsymbol{\Delta}\boldsymbol{\Theta}$, it can be proved, see Munthe-Kaas (1999); Iserles et al. (2000); Engø (2000),

$$\mathbf{d}\mathfrak{exp}_{\boldsymbol{\Theta}}^{-1}(\boldsymbol{\Delta}) = \boldsymbol{\Delta} - \tfrac{1}{2}[\boldsymbol{\Theta}, \boldsymbol{\Delta}] + \tfrac{1}{12}[\boldsymbol{\Theta}, [\boldsymbol{\Theta}, \boldsymbol{\Delta}]] + \ldots = \sum_{j=0}^{\infty} \frac{B_j}{j!}[\boldsymbol{\Theta}, [\boldsymbol{\Theta}, [\ldots, [\boldsymbol{\Theta}, \boldsymbol{\Delta}]\ldots]]], \tag{52}$$

where B_j are j'th Bernoulli numbers. The first few coefficients are

$$\frac{B_j}{j!} = \begin{cases} 0 & \text{for } k \text{ odd, and } k \neq 1 \\ 1, -\frac{1}{2}, \frac{1}{12}, -\frac{1}{720}, \frac{1}{30240}, -\frac{1}{1209600} & \text{for } k = 0, 1, 2, 4, 6, 8. \end{cases} \tag{53}$$

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References

Bhatia, R. (2007), *Positive definite matrices*, Princeton University Press, Princeton.

Engø, K. (2000), On the construction of geometric integrators in the RKMK class. *BIT*, Vol 40, No.1, pp 41-61.

Fiala, Z. (2011), Geometrical setting of solid mechanics. *Annals of Physics*, Vol 326, No.8, pp 1983-1997.

Fiala, Z. (2008), Geometry of finite deformations, linearization, and incremental deformations under initial stress/strain. In: *Engineering Mechanics 2008* (V. Fuis et al. eds). Svratka, CD ROM, paper #215, 20pp.

Fiala, Z. (2009), Is the logarithmic time derivative simply the Zaremba-Jaumann derivative? In: *Engineering Mechanics 2009* (J. Náprstek et al. eds). Svratka, CD ROM, paper, 14pp.

Hairer, E., Nørsett, S. P., Wanner, G. (1993), *Solving ordinary differential equations I: Nonstiff problems*, Springer, Berlin.

Iserles, A., Munthe-Kaas, H. Z., Nørsett, S. P., Zanna, A. (2000), Lie-group methods. *Acta Numerica*, Vol 9, pp 215-365.

Marsden, J. E., Ratiu, T. S. (1999), *Introduction to mechanics and symmetry*, Springer, New York.

Munthe-Kaas, H. (1999), High order Runge-Kutta methods on manifolds. *Applied Numerical Mathematics*, Vol 29, No.1, pp 115-127.

Noll, W., Seguin B. (2010), Basic concepts of thermomechanics. *Journal of Elasticity*, Vol 101, No.2, pp 121-151.