

# Bachelor-Thesis: Geometric integration on $SO(3)$

Dr. rer.nat. habil. Patrizio Neff and Dr. rer. nat. Kristian Debrabant

December 17, 2007

## 1 Introduction

In recent years, geometrical integration algorithms have become powerful tools for the long-time integration of nonlinear ode-systems. They are used, e.g., in the calculation of the trajectories of planets in our solar system. The key idea is to exactly preserve certain geometric properties of the analytical solution also within the numerical counterpart in order to improve dramatically the long-time accuracy of the solution [HLW06].

Here, we propose a bachelor-thesis project dealing with this issue in the context of a subproblem of a highly nonlinear continuum mechanical boundary value problem [Nef05, WN07, Nef03]. See also the poster in front of S215/405.

The task is, more precisely, to numerically integrate the system

$$\begin{aligned} \frac{d}{dt}R(t) &= \text{skew}[F(t)R^T(t)F(t)R^T(t) - 2F(t)R^T(t)] \cdot R(t) \\ R(0) &= R_0 \in SO(3), \quad F(t) \in GL^+(3), \\ \text{skew } X &:= \frac{1}{2}(X - X^T). \end{aligned} \tag{1}$$

It is easy to see that for given input history  $F \in C^1([0, T], GL^+(3))$ , the solution of (1) exists globally in time, and for all times  $R(t) \in SO(3)$ .

Moreover, if  $F$  is constant in time, then the scalar valued function

$$\begin{aligned} W(F, R) &= \|\text{sym}(R^T F - \mathbb{1})\|^2, \\ \text{sym } X &:= \frac{1}{2}(X + X^T), \quad \|X\|^2 := \sum_{i,j} X_{ij}^2, \end{aligned} \tag{2}$$

is decreasing along the flow, thus providing a Ljapunov function for (1).

## 2 Goal of the thesis

The student is assumed to implement and compare some numerical schemes (e.g. in Matlab or Mathematica) which preserve the geometric structure of the flow, i.e., in each time step

$t_n = t_{n-1} + \Delta t$  it is required to obtain  $R^n \in SO(3)$ . The scheme will in general be implicit and have the form

$$R^n = f(R^{n-1}, F^n, \Delta t), \quad F^n = F(t_n). \tag{3}$$

Further, the candidate should investigate the convergence properties of the scheme and establish the global attractor for the algorithm. Here, at fixed  $F$ , the flow will converge to a global minimum in  $R$  of (2), i.e.,

$$\lim_{n \rightarrow \infty} R^n = R_\infty \in \operatorname{argmin}_{R \in \operatorname{SO}(3)} W(F, R), \quad (4)$$

and these optimal rotations  $R_\infty^\pm$  are already known as a nonlinear function of  $F$ . This means that  $R_\infty^\pm = R_\infty^\pm(F)$  can be computed explicitly. Depending on initial conditions either  $R_\infty^+$  or  $R_\infty^-$  will be realized.

### 3 Requirements

The student should have a strong background in analysis and numerics of ordinary differential equations. We expect this project to last 8 weeks. At the end, the student will give a presentation in the seminar of 45 min., preferably in english and write a thesis of approximately 30 pages.

### 4 Continuation

The project can easily be adapted for Master-or Diploma thesis requirements, e.g., by additionally computing the so-called tangent of the scheme

$$D_{F^n} f(R^{n-1}, F^n, \Delta t), \quad (5)$$

which is needed in the coupling of the problem with FEM-solvers.

### References

- [HLW06] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations.*, second ed., Springer, Berlin, 2006.
- [Nef03] P. Neff, *Finite multiplicative plasticity for small elastic strains with linear balance equations and grain boundary relaxation.*, Cont. Mech. Thermodynamics **15** (2003), no. 2, 161–195.
- [Nef05] ———, *A geometrically exact viscoplastic membrane-shell with viscoelastic transverse shear resistance avoiding degeneracy in the thin-shell limit. Part I: The viscoelastic membrane-plate.*, Preprint 2337, <http://wwwbib.mathematik.tu-darmstadt.de/Math-Net/Preprints/Listen/pp04.html>, Zeitschrift Angewandte Mathematik Physik (ZAMP), DOI 10.1007/s00033-004-4065-0 **56** (2005), no. 1, 148–182.
- [WN07] K. Weinberg and P. Neff, *A geometrically exact thin membrane model-investigation of large deformations and wrinkling.*, Preprint 2500, <http://wwwbib.mathematik.tu-darmstadt.de/Math-Net/Preprints/Listen/pp07.html>, Technische Universität Darmstadt, Int. J. Num. Meth. Engrg., DOI: 10.1002/nme.2189 (2007).

#### Contact:

PD. Dr. Patrizio Neff  
 Fachbereich Mathematik, S215/405  
 Darmstadt University of Technology  
 Schlossgartenstrasse 7  
 64289 Darmstadt, Germany  
 email: neff@mathematik.tu-darmstadt.de

Dr. Kristian Debrabant  
 Fachbereich Mathematik, S215/321  
 Darmstadt University of Technology  
 Schlossgartenstrasse 7  
 64289 Darmstadt, Germany  
 email: debrabant@mathematik.tu-darmstadt.de