Mathematics in Facial Surgery

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This article deals with the role of mathematics in *cranio-maxillofacial surgery* (*cranium* = skull, *maxilla* = upper jaw), a special field of surgery focusing on patients with malformations of the upper and/or lower jaws or distinct bone defects, as shown in Figure 1. Operations include massive interventions like cutting of bones or relocation of bone segments up to several centimeters. Needless to say, such operations require extremely careful planning in advance, which is where mathematics comes in and, as will be shown, makes its crucial contribution.

Medical Planning Paradigm. In recent years, the following four-stage paradigm has crystallized (for a survey see [3]):

1. Given a *real patient* in the clinical situation.
2. Map this patient to the computer via medical imaging, thus generating a *virtual patient* in detailed individual 3D geometry.
3. Perform any medical planning in a *virtual lab*, which typically includes partial differential equation modeling and solving.
4. Play the results back to the *real patient* in the clinical situation.

Up to now, more than thirty clinical cases have been planned in close interaction with different clinics in Europe (Stage 1). Tomographic data, such as CT or MRI serve as input for Stage 2. The reconstruction of individual anatomic models from medical image data requires segmentation and 3D mesh generation—challenging mathematical topics of their own, which we are skipping here. Detailed information can be found in a recent survey [9]. Rather, we will concentrate on Stage 3, which involves the fast and reliable solution of PDEs from elasticity theory on the detailed 3D geometry of individual patients. The construction of virtual labs (here: `Facelab`) appeared to be crucial to make the information useful in the clinical environment. Finally, we compare our computational predictions with the individual patient outcome of the operations (Stage 4).

Biomechanical Model of Soft Tissue

Surgical relocation of bones induces associated facial tissue deformations, which characterize the facial appearance. In computer graphics and computer animation, the simulation of tissue deformations is often realized via so-called "mass spring models", compare, e.g., [5]. On one hand, such models provide immediate response, which is certainly a desirable feature in interactive surgery planning [7]. On the other hand, however, interactivity is obtained at the expense of numerical stability and approximation quality. At this point, mathematics enters and has to share part of the

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medical responsibility. In fact, a *reliable* preoperative prediction of the expected postoperative facial appearance on the basis of a detailed *individual* mathematical model is of vital importance for any patient.

In mathematical terms, soft tissue deformation can be described by a mapping $\phi : \Omega \to \mathbb{R}^3$ from the undeformed reference domain $\Omega \subset \mathbb{R}^3$ to its deformed counterpart $\Omega' \subset \mathbb{R}^3$. Usually, computations are performed in terms of the *displacement* $u = \phi - I$. The relocation of bones prescribes a certain displacement on the Dirichlet interface $\Gamma_D \subset \partial\Omega$ of bone and soft tissue. Soft tissue may be modelled as a *hyperelastic material*, admittedly a simple model which, however, yields surprisingly good results. In this model, the deformation is given by minimizing the stored energy

$$f(\phi) = \int_\Omega W(\nabla\phi)\, dx.$$

Different material behavior is due to different *material laws* W. The most widely used law is the linear St. Venant-Kirchhoff material

$$W(\nabla\phi) = \frac{\lambda}{2}(\mathrm{tr}\varepsilon)^2 + \mu\,\mathrm{tr}\varepsilon^2$$

depending on the linearized Green-Lagrange strain tensor

$$\varepsilon = \frac{1}{2}(\nabla u^T + \nabla u)\,.$$

This model leads to a convex quadratic stored energy f, and hence to the linear Lamé-Navier equation

$$\begin{aligned} -2\mu\,\mathrm{div}\varepsilon - \lambda\nabla\mathrm{div}u &= 0 && \text{in } \Omega \\ u &= u_0 && \text{on } \Gamma_D \\ 2\mu\varepsilon + \lambda\,\mathrm{tr}\varepsilon I &= 0 && \text{on } \partial\Omega\backslash\Gamma_D. \end{aligned}$$

In [10], the two constants describing the St. Venant-Kirchhoff material law have been identified from postoperative results. The obtained values of Young's modulus E and the Poisson ratio ν are $\mathsf{E}_m \geq 300\text{kPa}$, $\nu_m \approx 0.44$ for muscle and $\mathsf{E}_s \leq 50\text{kPa}$, $\nu_s \approx 0.46$ for embedding soft tissue. From these values, the parameters

$$\lambda = \frac{\mathsf{E}\nu}{(1+\nu)(1-2\nu)}\,, \quad \mu = \frac{\mathsf{E}}{2(1+\nu)}$$

can be computed for $\nu < 0.5$. In numerical sensitivity studies we found out that any choice of the Poisson ratio between 0.3 and 0.47 supplied more or less the same results.

The above linear material law is known to be insufficient for large compressive strains and rotations (see, e.g., [6]) as they occur in surgery planning. In particular, interpenetration of the material may occur, unless the stored energy satisfies

$$(1) \qquad W \to \infty \quad \text{for} \quad \det\nabla\phi \to 0.$$

Figure 1. Patients with facial malformations.

Such physically reasonable material laws are necessarily *nonconvex*, which plays a role both in the existence theory requiring Ball's concept of polyconvexity and in the computational approach, see below.

A simple polyconvex material law of the Ogden type satisfying (1) has been derived by Ciarlet and Geymonat [1, §4.10] as

$$\begin{aligned} W(\nabla\phi) &= W(I + \nabla u) \\ (2) \qquad &= a\,\mathrm{tr}E + b(\mathrm{tr}E)^2 + c\,\mathrm{tr}E^2 + d\Gamma(\det(I + \nabla u)), \end{aligned}$$

depending on the full Green-Lagrange strain tensor

$$(3) \qquad E = \frac{1}{2}(\nabla u^T + \nabla u + \nabla u^T \nabla u)\,.$$

Observe that here the geometric nonlinearity comes in. The most appealing feature of the above material law is that with

$$\begin{aligned} a &= -d\Gamma'(1), & b &= \frac{1}{2}(\lambda - d(\Gamma'(1) + \Gamma''(1))), \\ c &= \mu + d\Gamma'(1), & d &> 0, \qquad \Gamma(s) = s^2 - \ln s, \end{aligned}$$

near the undeformed reference state it is a second-order approximation to the linear St. Venant-Kirchhoff material to λ and μ, which is recovered asymptotically for $d \to 0$.

Affine Conjugate Adaptive Newton Methods

The problem to be solved numerically is the minimization of the nonlinear stored energy

$$(4) \qquad f(u) = \int_\Omega W(I + \nabla u)\, dx\,,$$

wherein the nonlinearity originates both from the material law (2) and the Green-Lagrange strain tensor as defined in (3). This functional is dominantly convex with non-convex insertions as indicated above. A necessary condition is $F(u) = f'(u) = 0$, which is just the PDE system modeling nonlinear elasticity. If, in addition, $F'(u) = f''(u)$ is *strictly positive definite*, then there exists a unique local minimizer.

In the purely *convex* case, affine conjugate Newton methods would certainly be among the efficient methods for its solution. The basic idea behind this class of methods (see the recent monograph [4]) is to regard the functional as just one representative out of all possible functionals $g(v) = f(Bv)$ generated by arbitrary linear bijective transformations B. This transformation would lead to

$$G(v) = F(u)B = f'(u)B = 0$$

and to

$$G'(v) = B^*F'(u)B = B^*f''(u)B,$$

all positive definite due to the standard conjugacy argument (hence the name).

Let the *damped Newton iteration* ($k = 0, 1, \dots$) be defined by

$$F'(u^k)\Delta u^k = -F(u^k),$$
$$u^{k+1} = u^k + \lambda_k \Delta u^k\,,$$

with damping factor $\lambda_k \in]0, 1]$. Of course, the aim is to achieve iterative *functional decrease*

$$f(u^{k+1}) < f(u^k)\,.$$

With $\|\cdot\|$ denoting the L_2-norm, nonlinearity may be characterized via an affine conjugate Lipschitz condition

$$\|F'(u)^{-1/2}(F'(w) - F'(u))(w - u)\| \le \omega\|F'(u)^{1/2}(w - u)\|^2$$

in terms of a Lipschitz constant ω, which is obviously independent of any choice of B. With the further definitions

$$\epsilon_k = \|F'(u^k)^{1/2}\Delta u^k\|^2\,, \quad h_k = \omega\|F'(u^k)^{1/2}\Delta u^k\|$$

for the local energy norms ϵ_k and the corresponding Kantorovich quantities h_k, the functional decrease can be analyzed in terms of the *cubic upper bound*

$$f(u^k + \lambda\Delta u^k) \le f(u^k) - t_k(\lambda)\epsilon_k$$

with

$$t_k(\lambda) = \lambda - \frac{1}{2}\lambda^2 - \frac{1}{6}\lambda^3 h_k\,.$$

For this estimate, the optimal choice of damping factor comes out as

$$\overline{\lambda}_k = \frac{2}{1 + \sqrt{1 + 2h_k}} \le 1\,.$$

For the realization of an *adaptive* Newton algorithm, corresponding computational estimates $[\omega] \le \omega$, also affine conjugate, are conveniently obtained in the course of computation and exploited to control the iteration. In other words, the unavailable Kantorovich quantities h_k are replaced by computationally available estimates $[h_k] \le h_k$ and, consequently, the theoretical damping factor $\overline{\lambda}_k$ by the value

$$[\overline{\lambda}_k] = \frac{2}{1 + \sqrt{1 + 2[h_k]}} \le 1\,.$$

Of course, since $[h_k] \le h_k$, we have $[\overline{\lambda}_k] \ge \overline{\lambda}_k$ so that a prediction step must be possibly followed by additional correction steps. In [4], this type of method has been worked out for levels of increasing algorithmic complexity: exact, inexact, and function space oriented Newton methods. The latter class of methods represents the theoretical frame needed to develop *adaptive multilevel finite element methods* for PDEs, which is our context here.

In [8], this idea has been extended to the *non-convex* case arising in nonlinear biomechanics, where $F'(u_k)$ may be indefinite or even singular as indicated above. As a consequence, the Newton direction, even if it exists, need no longer be a functional descent direction, and $F'(u_k)$ need not induce an energy norm. Therefore, the above definition of ω no longer makes any sense. Fortunately, however, in the case of biomechanics, there is a natural decomposition

$$F'(u_k) = M + N(u_k)$$

where $M = F'(0)$ represents the positive definite *linear* elastomechanics part and

$$N(u_k) = \mathcal{O}(\|\nabla u_k\|) \text{ for } \|\nabla u_k\| \to 0$$

comprises the nonlinearity. Hence, M induces a convenient energy norm $\|\cdot\|_M = \|M^{1/2}\cdot\|$, which again is independent of B, giving rise to an affine conjugate Lipschitz condition of the form

$$\|M^{-1/2}(F'(w) - F'(u))(w - u)\| \le \omega\|M^{1/2}(w - u)\|^2\,.$$

With this notation, we may rewrite the above cubic upper bound as

$$f(u^k + \delta u^k) \le f(u^k) + \theta_k(\delta u, \omega)\,.$$

with

$$\theta_k = \langle F(u_k), \delta u_k\rangle + \frac{1}{2}\langle \delta u_k, F'(u_k)\delta u_k\rangle + \frac{\omega}{6}\|\delta u_k\|_M^3\,.$$

The corrections δu are understood to vary within a low-dimensional subspace δU_k; in the purely convex case above, this subspace is one-dimensional with $\delta U_k = \mathbb{R}\delta u_k$ and δu_k an inexact Newton correction obtained, e.g., from preconditioned conjugate gradients (PCG). In the non-convex case, the

PCG will terminate as soon as a direction of negative curvature, say p_k, is encountered; then δU_k will include p_k. Proceeding like this has been inspired by techniques established in finite but high-dimensional nonlinear programming [2]. Given this subspace, we proceed as in the convex case: we replace the Lipschitz constant ω by its computational estimate $[\omega]$ and determine the iterative correction from the low-dimensional minimization problem

$$\delta u_k = \arg \min_{\delta w \in \delta U_k} \theta_k(\delta w, [\omega]) .$$

In actual computation, the infinite-dimensional minimization problem $f(u) = \min$ must be discretized. In order to preserve as much of the original problem's structure as possible, we aim at a multilevel finite element discretization to be realized on a sequence of 3D grids, adaptively refined by means of a posteriori error estimates. These estimates also enter into the control of the inexact Newton multilevel finite element iteration.

In passing we note that the above mentioned "mass spring models" may be regarded as an ad hoc discretization of a not-well–specified linear elasticity PDE model.

Computational Predictions versus Surgical Results

In close cooperation with surgeons, we have computed a number of patient cases on the basis of the above biomechanical model and by means of the described adaptive Newton algorithms.

A *qualitative* comparison of our predictions with postoperative results documented by profile photographs, already yields a surprisingly good correspondence. As an example, Figure 2 shows a pre- and a postoperative image as well as an overlay view of the predicted 3D facial tissue (semitransparent) with relocated bony structures (opaque) and the photograph of the final outcome. Clearly, such an evaluation allows for a comparison of the soft tissue *profile* only.

More detailed *quantitative* three-dimensional comparisons have been conducted using pre- and postoperative tomographic image data [10]. Note that the actually performed operation may not be identical with the planned one. For this reason, we aimed at a virtual reproduction of the actual surgical procedure to arrive at the real postoperative bone locations starting from preoperative data. The pre- and the postoperative models were aligned via the neurocranium, which had not been affected by the surgical procedure, using an iterative closest point method. The mean alignment error came out to be of the order of 0.1–0.2 mm. Afterwards, mobile bone segments (like the mandible, the hyoid, and the spine as well as the osteotomized maxilla) were rigidly aligned via anatomic landmarks. Here, the alignment error of the two bony skulls arose

Figure 2. Patient before (left), and after operation (center), overlay with computed prediction (right).

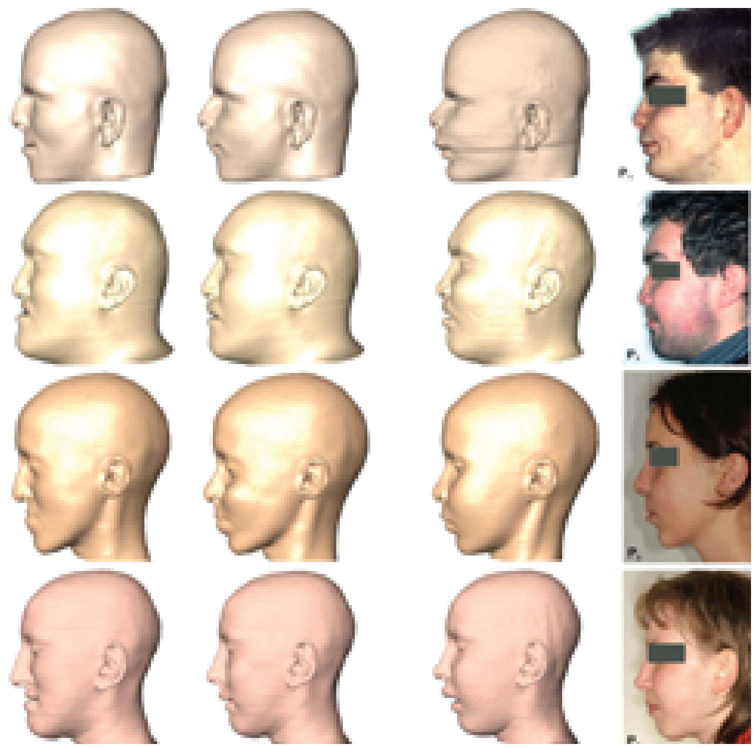

Figure 3. Predicted versus real postoperative results for four patients: 3D reconstruction from preoperative CT data (left), simulation after surgery planning (center left), reconstruction from postoperative CT data (center right), and postoperative photograph (right).

as less than 0.5 mm, measured as the Hausdorff distance between pre- and postoperative bone surfaces.

Once the bone alignment has been realized as described, a comparison of soft tissue deformations was possible. In view of a meaningful quantitative evaluation, we decided not to consider the entire head, but only the facial region, which is affected by the surgical operation. Approximately 70% of the facial skin surface shows a prediction error below 1 mm, and only 5–10% exhibit a deviation larger than 3 up to 3.8 mm. These areas were underestimated

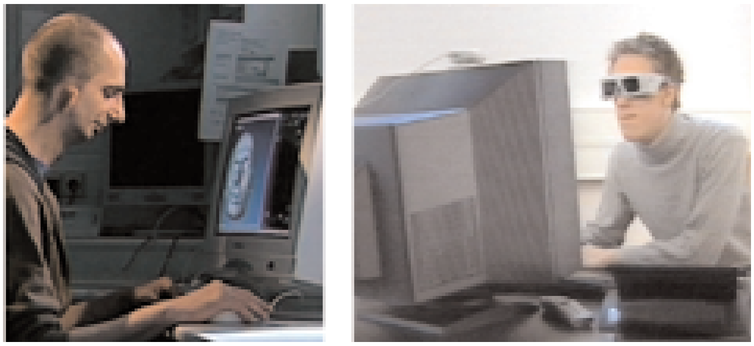

Figure 4. Improved preoperative patient information.

mainly due to postoperative swelling. However, in maxillofacial surgery planning, a mean prediction error of about 1–1.5 mm seems to be a fully acceptable result.

Figure 3 shows the results for four patients (with distinct midfacial hypoplasia and class III dysgnathia), where a maxillary advancement of up to 15 mm had been planned and executed.

Impact

Even though biomechanical tissue modeling turns out to be a tough problem, we are already rather successful in predicting postoperative appearance from preoperative patient data. For the surgeon, our computer assisted planning permits an improved preparation before the actual operation. Different operation variants can be studied in advance and evaluated. For patients, our planning clearly leads to better preoperative information and therefore an improved decision basis. Some patients even actively participated by using our planning system themselves (see Figure 4). Moreover, our methods also contribute to a detailed documentation and quality assurance as well as to surgical education and training. In particular, new or unconventional osteotomy techniques can be simulated on *virtual* patient models. Thus mathematics also helps fostering surgical progress.

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