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# Negative Jacobian free simulations using principal stretches

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**Abstract**

*Finite element (FE) simulations are prone to encountering negative Jacobians during the solving process. If nothing is done, the simulation can be brought to a halt, result in inverted elements or have undetermined behavior. We propose a solution that uses principal stretches as slack variables in a constrained minimization formulation and enforce them to always be positive. We show that our approach can never hit inverted configurations, thus being suitable for applications where inversion cannot be tolerated. We implement the method in 2D and show that it outperforms standard FE methods in stressful scenarios.*

**CCS Concepts**

• ***Computing methodologies*** → ***Physical simulation;***

## 1. Introduction

Elasticity FE problems are typically solved using the Newton method or other nonlinear unconstrained optimizers. But any of these solvers can overshoot into domains where the elements are inverted. This is a problem as the behavior of the elastic material is often undefined in that region. Ideally, we would like inversion to never happen during the solving process. Here, we focus on adding constraints to the minimization that prevent inverted elements altogether. These can be constraints on the Jacobian of the deformation gradient $J > 0$ or on the principal stretches $s_i > 0$. Enforcing the additional constraints (like in *strain limiting*) can work, but many solvers do not enforce strict feasibility at every step. This is why we chose to express these constraints as slack variables together with additional equality and bounds constraints on them. We also chose to use principal stretches $s_i$ over $J$ as slack variables, due to the ambiguity in the deviatoric-volumetric split of the energy, especially for coupled materials like compressible Neo-Hookean. For isotropic materials, one can express the whole energy function in terms of principal stretches and the only part of the total energy left is the work of the external and inertia forces.

There is a lot of work in the graphics community on inversion [ITF04, SHST12], but these allow for inversion to take place and then recover from it. Many authors prefer to use principal stretches formulations of FE elasticity, among which are mixed formulations. In fact, our method can be shown to be a full stress three field mixed formulation [BW97]. Moreover, at a closer inspection *projective dynamics* can be viewed in the same way. The work of [NOB16] implements a prox operator in terms of principal stretches that is very similar to our approach. However, to the best of our knowledge, our formulation is the first one that uses the principal stretches as explicit variables and focuses on the inversion problem.

## 2. Problem formulation

Most static FE elasticity problems can be expressed after discretization as the unconstrained problem of minimizing the objective $U(\mathbf{x}) + E(\mathbf{x})$, where $U$ is the elastic potential and $W$ is the work of the external forces (body loads and Neuman boundary conditions). The gradient of the objective and the optimality conditions are given by $\nabla U(\mathbf{x}) + \nabla E(\mathbf{x}) = -\mathbf{f}_{int}(\mathbf{x}) - \mathbf{f}_{ext}(\mathbf{x}) = 0$. The external forces are often constant (e.g. gravity or constant loads), in which case $E = -\mathbf{x}^T \mathbf{f}_{ext}$ and has a zero Hessian. We will be focusing on linear triangle elements in this paper and gloss over many continuum mechanics and FE details, which can be found in [BW97]. The deformation gradient $\mathbf{F}$ of a triangle $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ is a function of the nodal positions $\mathbf{x}$ through the relation $\mathbf{F} = \mathbf{D}_s(\mathbf{x})\mathbf{D}_m^{-1}$, where the $\mathbf{D}$ shape matrices have the form $[\mathbf{x}_2 - \mathbf{x}_1 \ \mathbf{x}_3 - \mathbf{x}_1]$ evaluated at the current (spatial) and initial (material) configurations. The principal stretches $\bar{s}_i$ are defined as the singular values of $\mathbf{F}$. These values are computed for each element by performing a singular value decomposition (SVD): $\mathbf{F}(\mathbf{x}) = \mathbf{U}\Sigma\mathbf{V}^T$, where $\Sigma = \mathrm{diag}(\bar{s}_i)$ and $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices.

We now formulate a constrained minimization problem that uses the additional slack variables $\mathbf{s}$:

$$\min_{\mathbf{x},\mathbf{s}} E(\mathbf{x}) + U(\mathbf{s}) \ \text{ s.t. } \bar{s}_i^e(\mathbf{x}) - s_i^e = 0, s_i^e \geq 0. \tag{1}$$

We use a special version of the SVD that contains only pure rotations (no reflections). This means that they are first allowed to take negative values that would indicate an eventual inversion and then enforced to always be positive by the additional constraint. In order to obtain such signed values we need to slightly modify the SVD so that it always outputs rotation matrices. Such a procedure is described by [ITF04] and others, who negate the necessary columns in $\mathbf{U}$ and $\mathbf{V}$ and the smallest singular value if needed.

## 3. Numerical implementation

The problem in (1) can be solved with any solver that can handle nonlinear equality constraints and simple bounds constraints. However, we would like to devise an algorithm that is custom built. This is why we chose the *alternating direction method of multipliers* (ADMM) [NOB16], given the separable nature of the problem. Another solver we devised is based on solving the nonlinear equations resulting from the Karush-Kuhn-Tucker (KKT) optimality conditions. Most nonlinear equation solvers rely on some form of the Newton method and this is why we call it a Newton solver.

Most optimization algorithms require the gradient of the objective and that of the constraints. The gradient of the objective is made of $\nabla E = -\mathbf{f}_{ext}$ and $\partial U/\partial \mathbf{s}$ which can be computed from the isotropic energy density expressed in principal stretches. The Lagrangian of the problem in (1) is $L(\mathbf{x},\mathbf{s},\eta) = E(\mathbf{x}) + U(\mathbf{s}) + \eta^T \Phi(\mathbf{x},\mathbf{s})$, where $\eta$ are Lagrange multipliers related to the second Piola-Kirchoff tensor. The resulting KKT optimality equations are

$$\frac{\partial E}{\partial \mathbf{x}} - \frac{\partial \bar{\mathbf{s}}}{\partial \mathbf{x}}^T \eta = 0,\ \frac{\partial U}{\partial \mathbf{s}} + \eta = 0,\ \Phi(\mathbf{x},\mathbf{s}) = 0. \tag{2}$$

Some solvers require the Hessian w.r.t. $\mathbf{x}$ and $\mathbf{s}$ of the Lagrangian $\mathrm{diag}\left(-\frac{\partial^2 \bar{\mathbf{s}}}{\partial \mathbf{x}^2}\eta, \frac{\partial^2 U}{\partial \mathbf{s}^2}\right)$. We give without proving the formula $\partial \bar{s}_i/\partial \mathbf{x}_j = \mathbf{r}_j^T \mathbf{v}_i \mathbf{u}_i$, where $\mathbf{r}_j^T$ are the rows of $\mathbf{D}_m^{-1}$ for $j = 1,2$, $\mathbf{r}_1 = -\mathbf{r}_2 - \mathbf{r}_3$, and $\mathbf{u}_i$ and $\mathbf{v}_i$ are the columns of $\mathbf{U}$ and $\mathbf{V}$. One thing to note here is that the SVD is not unique when the singular values are equal. On the other hand, the singular values are continuous at such points and their derivatives are unique. This is why we are not using finite difference approximations. A different story applies to the Hessian of $\bar{\mathbf{s}}$ as it includes gradients of $\mathbf{U}$ and $\mathbf{V}$ which are not unique or continuous. Although semi-analytical recipes exist [SHST12], we chose to compute the Hessian of the Lagrangian w.r.t. $\mathbf{x}$ using finite differences.

ADMM separates the problem into a sequence of two subminimizations: one for $\mathbf{x}$ and one for $\mathbf{s}$. The former is an unconstrained one, while the latter has very simple bounds constraints. The scaled version of ADMM at the $k$th iteration has the form:

$$\mathbf{s}_{k+1} = \arg\min_{\mathbf{s}\geq 0} U(\mathbf{s}) + \frac{\rho}{2}\|\Phi(\mathbf{x}_k,\mathbf{s}) + \mathbf{u}_k\|_2^2, \tag{3a}$$

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{x}} E(\mathbf{x}) + \frac{\rho}{2}\|\Phi(\mathbf{x},\mathbf{s}_{k+1}) + \mathbf{u}_k\|_2^2, \tag{3b}$$

$$\mathbf{u}_{k+1} = \mathbf{u}_k + \Phi(\mathbf{x}_{k+1},\mathbf{s}_{k+1}), \tag{3c}$$

where $\rho$ is a penalty factor and $\mathbf{u} = \eta/\rho$ are the scaled Lagrange multipliers. The gradient of the $\mathbf{x}$ minimization objective is $\nabla \bar{E} = -\mathbf{f}_{ext} + \rho \nabla \bar{s}(\Phi + \mathbf{u})$. For the minimization in $\mathbf{s}$ we can use a projected gradient sub-minimizer: $\mathbf{s}_{n+1} = \max(0, \mathbf{s}_n - \alpha \nabla_{\mathbf{s}} \bar{U}(\mathbf{s}_n))$, where $n$ indicates the iteration number, $\nabla_{\mathbf{s}} \bar{U}(\mathbf{s}_n) = \nabla_{\mathbf{s}} U(\mathbf{s}_n) + \rho(\Phi(\mathbf{x},\mathbf{s}_n) + \mathbf{u})$ and $\alpha$ is the step length. As you can see we have at least two iterative methods nested into one another and lots of parameters for them: $\rho$, $\alpha$ and the maximum number of iterations. You are guaranteed at every step that no inverted configurations will be reached given $s_i$ are always positive. In our experiments we have found $\rho = 10^9$, $\alpha = 10^{-10}$ to work well. In addition, we used convergence criteria to early terminate the iteration. For gradient descent we used as a measure the relative change of the norm of the gradient. We used a relative tolerance for ADMM too, but this time we applied it to the $\ell 1$ merit function $\phi_1(\mathbf{x}) = E(\mathbf{x}) + U(\mathbf{s}) + \rho(\max_i |u_i|)\|\Phi(\mathbf{x},\mathbf{s})\|_1$. For our experiments, we used a relative threshold of $10^{-7}$ for the merit function in conjunction with a $10^{-4}$ absolute threshold for $\|\Phi\|_2$.

The Newton solver is essentially one that solves the nonlinear equations in (2) without considering the bounds constraints while using Hessian information. In practice, we found that the system in (2) without the bounds constraints is enough to solve the problem without running into inverted configurations. As for the inequality bounds constraints, we resorted to the remapping $\mathbf{s} = \exp(\sigma)$ and used $\sigma$ as a variable instead of $\mathbf{s}$. This prompted the recalculation of the gradients and Hessian w.r.t. $\sigma$: $\frac{\partial U}{\partial \sigma} = \mathcal{S}\frac{\partial U}{\partial \mathbf{s}}$, $\frac{\partial^2 U}{\partial \sigma^2} = \mathrm{diag}\left(\mathcal{S}\frac{\partial U}{\partial \mathbf{s}}\right) + \mathcal{S}\frac{\partial^2 U}{\partial \mathbf{s}^2}\mathcal{S}$, where $\mathcal{S} = \mathrm{diag}(\mathbf{s})$. By replacing these into (2) and the Hessian we are able to solve the modified nonlinear equations that also satisfy the inequality constraint in (1). Using the above substitution and the gradient expression, we can also derive an exponential map form of gradient descent: $\mathbf{s}_{n+1} = \mathbf{s}_n \exp[-\alpha \mathbf{s}_n \nabla_{\mathbf{s}} \bar{U}(\mathbf{s}_n)]$, that can be used instead of the projected gradient descent in the ADMM solver.

## 4. Results and conclusions

We have implemented these solvers in Matlab. One of the main experiments we made was to compress a bar as we found it to be a hard problem to solve. The standard method is always in danger of inverting and starts giving unrealistic solutions under stress, the only surviving solvers being our ADMM and Newton solvers, as depicted in Figure 1 of the accompanying material. In Figure 2 we fixed the bar by both ends and applied a vertical load on top. The triangles become very thin, but a solution is still possible without encountering inversion. In conclusion, we introduced a constrained minimization framework using principal stretches that avoid element inversion. We devised two solvers and extended them with an exponential map that guarantees positive principal stretches. We are currently working on a C++ version that does not rely on any external library, as well as an extension to 3D.

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