Title:
Estimation of Surface Stresses on Voxel Meshes by FEA and Neuronal Nets in 2D Plane Stress Models

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Introduction:

This work targets the integration of structural FEA into machine learning processes. While the former traditionally relies on meshes specifically constructed for the geometry under consideration, the latter typically make use of voxel meshes to represent geometry. Applying FEA on voxel meshes is possible, computationally advantageous and will give meaningful results in terms of displacements, but suffers a limitation: Calculating stresses directly and locally from the displacement results of FEA typically gives unsuitable results due to the jagged nature of the mesh. Therefore, for problems characterized by critical stress values, an additional model for obtaining stress estimates from displacement results is needed.

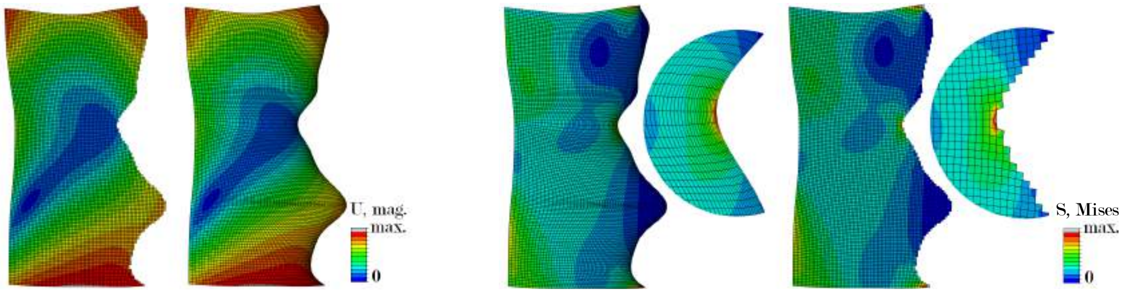
This work, as a first step, suggests and demonstrates a method for constructing such a model in an heuristical way, specifically by training a neuronal net, for two-dimensional plane stress problems. Despite the fact that, thereby, the term “Pixel” should be more accurate, “Voxel” will be used in reflection of the larger-scale intentions.

Voxel-style meshes are a natural choice for several types of analyses, particularly in the context of optimization methods: Many machine-learning methods operating on geometric data (specifically those incorporating convolutional networks) operate on such representations [2]. In addition, CT-type scans of natural structures like trabecular bone naturally yield voxel-style representations of specimens [4].

While stiffness may be the relevant criterion for many mechanical engineering problems, others are guided by strength as the main guiding factor. For some of such problems, fatigue behavior may be modeled based on strains [3], in particular for biological materials. In contrast, for many engineering materials, the accurate calculation of local surface stresses is a necessity. Particularly in a high cycle fatigue context, stress results on a component’s model’s surface may be an essential (and even sufficient) basis for modeling fatigue behavior.

On a voxelized representation of geometry, though, calculating stresses is not immediately possible in a meaningful way: Element stress results recovered from FEA results may be distorted by the choice of edge length and even coordinate origin rather than reflecting the implied underlying geometry accurately. Surface stresses will not converge with usual finite element formulations due to the jagged nature of the model. In contrast, displacement results convergence with small element size and are consistent with results from smooth meshes (see figure 1a compared to figure 1b).

One obvious strategy for calculating stresses is to derive an estimation of the underlying (smooth) geometry, meshing this geometry suitably and performing FEA on this new mesh. With this strategy,



(a) Displacement Results (magnitude) (b) Stress Results (von Mises)

Fig. 1: Results from one Sample Problem, on both smooth and voxelized Models

known implementations of the smoothing and re-meshing step will impede the backtraceability of the overall process. Many optimization algorithms, particularly those frequently used in machine learning, though, benefit from the availability of exact gradients. For many applications of FEA as well as neuronal nets, the calculation of the respective outputs' gradients with respect to the elements' stiffness (i.e., the voxels' presence in the model) is known. Consequently, a stress calculation based on the voxel mesh can benefit such algorithms.

Applications for a voxel-based approach that could be the machine-learning-based design automation processes combining previously learned features in complex ways[5]. In the context of biomimicry, that is the transfer of patterns from natural systems like the above mentioned trabecular structures onto technical ones, such calculations may offer benefit in integrating natural patterns with artificial systems.

Generation of Reference Problems

To provide a sufficient data basis for training a heuristic model, a parametrized class of problems was defined. It was constructed as follows: each training problem is based on a gridded mesh of square quadrilateral elements. The total width of the base mesh is 0.5 and its height is 1.0. While the other three edges of this mesh remain fixed, the right edge of each sample is distorted according to the following class of function. An example mesh can be seen in figure 1. Let y be the vertical coordinate in this representation and the center point of the original right edge (that is to be distorted) the origin of the coordinate system. Then the function (representing a Fourier series)

$$s(y) = c\sum_{i=1}^{n} a_i q^i \sin\left(\frac{iy}{2\pi} + \varphi_i + \varphi_0\right) \qquad (c, n, q) = (0.2, 10, 0.5)$$

gives the boundary of the deformed patch for $y \in [-0.5, 0.5]$. The parameters $\varphi_i \in [0, 2\pi[$ and $a_i \in [0, 1[$ were chosen randomly for each sample. Subsequently, φ_0 was adjusted so that $s(-0.5) = s(0.5) = 0$. Bi-linear plane stress quadrilateral elements were used in FEA.

In close analogy to the randomly generated geometry, random boundary constraints were defined in suitable polar coordinates for all points on the undeformed three edges. In addition, constant terms enabling omnidirectional strain were introduced. Figure 1a shows the displacements calculated for such a randomly generated sample problem. As stiffness of the models coincide (assuming sufficiently small edge lengths in the voxel model), the interior displacement values show very good consistence.

In contrast, surface stress results in the voxelized model may not be interpreted meaningfully, as shown in figure 1b.

Extraction of Training Data:
Subsequently, for every sample problem, for every sufficiently interior (i.e. distant from any boundary constraints) voxel at the deformed edge, an input dataset and target stress data were extracted: binary "density" as well as 2-D displacements from the surrounding 15-by-15 voxel patch (16-by-16 nodes) were used as input data, suitably preprocessed stress tensors served as target values. Via rotation, every such sample effectively provided four pieces of data for training.

As a neuronal net was only to used to model the non-linear effects of the problem, the following three-step normalization process was used:

- Removing rigid body rotations: This was also a prerequisite for meaningful scaling of displacements (last step). Small rotations were assumed, so rotating the stress values could be neglected.
- Centering: The displacement values were offset so that the arithmetic mean value was be zero.
- Displacement scaling: The displacement values were scaled so that the quadratic mean value was equal to 1. This – in contrast to the two previous steps – requires the consistent scaling of the stress values.

This way, the model could be trained to return a dimensionless stress factor independent on voxel resolution and material (neglecting effects of Poisson's ratio, which was set to 0.3).

To investigate the influence of the "range of perception" of the model, this preprocessing of data was performed for several sub-sets of the original 16-by-16 data-sets. In the following, n_d and n_u shall denote the "radii" of the density input field and displacement input, respectively.

Training of the Model:
Based on the maximum number of input channels of 768 and some initial experiments, the following architecture of the neuronal net was used as a basis: Two hidden layers of dimension 128 and 64 were used. All hidden layers were fully connected with their predecessor and made use of tanh-activation and a bias vector. The output layer naturally was of dimension 3 and used identity as activation. To investigate the complexity of the problem, two additional nets were investigated which resulted from inserting a layer of size 256 to the input side or removing the layer of size 128 from the net described above without changing any other characteristics.

Training was performed using a stochastic gradient descent algorithm incorporating a momentum term. The loss function was defined as the mean square error with respect to the the plane stresses as a vector.

Verification loss values (with respect to sample problems not used for training) are given below, together with the total number of degrees of freedom in the model.

	DOFs at $(n_\mathrm{d}, n_\mathrm{u}) =$			Losses at $(n_\mathrm{d}, n_\mathrm{u}) =$		
Hidden Layer Sizes	(8,8)	(8,4)	(4,4)	(8,8)	(8,4)	(4,4)
256,128,64	238 211	139 907	90 755	0.00270	0.00369	0.00513
128,64	106 883	57 731	33 155	0.00283	0.00364	0.00516
64	49 411	24 835	12 547	0.00292	0.00376	0.00523
lin. reg.	2 307	1 155	579	0.0129	0.0129	0.0129

These results show very little dependency on model complexity, that is, even the simplest models gave reasonably accurate results. This indicates that the problem of estimating stresses on sufficiently smooth underlying geometries is much simpler than initially expected. For reference, the results of a linear regression model on the same data-set is given in the last line.

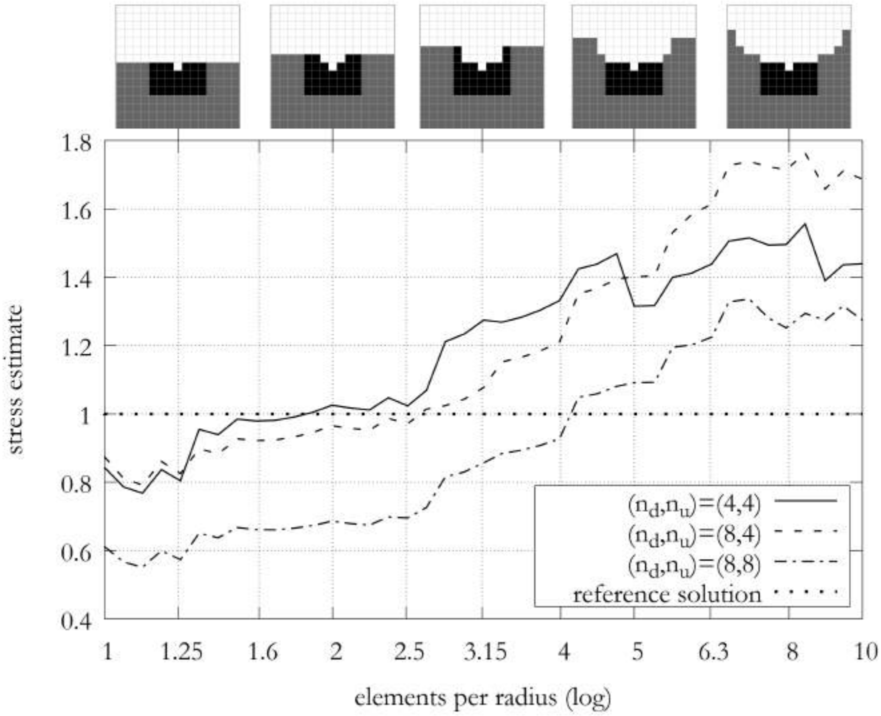


Fig. 2: Results for the notched Beam

Verification:

Outside-model validation was attempted to investigate the suitability of the proposed process for real-world engineering problems. A beam with a circular notch under torsional loading was chosen, as it exhibits particularly significant differences to the problems within the training data set: Instead of the harmonic nature of the training data defined by a finite Fourier series, it consists of segments of constant curvature, connected by sharp corners. Still, in principle, it should be possible to estimate the curvature – and thereby the stress values – within those segments assuming the choice of a suitable resolution.

The voxelized model investigated below was constructed so that at the critical location (i.e. the center of the notch), there was always a gap exactly one voxel wide. This choice was made in order to provoke possible artifacts of the models, thereby serving as a plausible worst-case problem. The lower part of figure 2 compares the (von-Mises-equivalent) stress estimates of the models.

The results show a strong dependence of the model output on the voxel resolution. The monotonic nature of the dependency was to be expected: Higher resolutions will allow for a more precise estimation of curvature, while for low resolutions, the surrounding segments of curvature 0 will dominate.

For context, the upper part of figure 2 shows the scope of input for selected models (resolution indicated by the tick marks connecting the grids to the plot). Black cells are parts of the area of “radius” 4, gray cells of the area of “radius” 8. White cells are not part of the model.

The curves for the $n_u = 4$ seem to show a plateau for 1.5 to 2.5 elements per radius in good accordance with the reference solution. This should not be overstated, as in this range the notch is represented by a constant voxel mesh and differences in model output only result from slight differences in the displacement field.

While underestimation of stresses at low resolutions directly results from the smoothness of training problems, the overestimation at high resolutions is less obvious: For high resolutions, the problem gives the same geometric input for very high and very low resolutions (a straight boundary with one voxel missing). Normalized strain will vary at a different rate within the geometry, but this effect is dominated by overall bending stiffness (i.e. relative width) rather than any property of the notch itself. The model thereby can not distinguish those situations from each other and will return a very similar factor > 1 for both problems (approximately 1.7 for $(n_\mathrm{d}, n_\mathrm{u}) = (8, 8)$). Both problems being close to a straight edge, the reference stress (explicitly given in the full paper) could be informally described as the "average stress" in the geometry under consideration. For low resolutions, this reference stress gives a value close to the "nominal stress", which is to be scaled by a concentration factor in classical mechanical engineering. For high resolutions, in contrast, the surface stress in the voxel model is already very close to the real stress at the center of the notch. This very effect had not been observed in the training problems due to the limited range of included harmonics.

Judging from these overall results (on a particularly adverse problem), the models trained in this work are not yet suited for engineering applications due to their limited accuracy.

Conclusion

The proposed method resulted in a heuristical model that gave precise results within the class of problems used for training. Unfortunately, the model of problems based on Fourier series turned out insufficient to cover some engineering problems.

Further research will utilize tools built within this work and will be targeted at:

- Enriching the training data by redesigning the model of training problems: This could either be done by adding broader frequency content or (potentially non-differentiable) non-harmonic functions to the basis that consisted of harmonic functions in this work's approach. Alternatively, contours could be generated by combining defined parametrized features.
- A systematic investigation into the (implicit) assumptions of a heuristic model depending on the model (and parameter values) of training problems.
- A transfer of a promising method onto 3-D problems.

Ultimately, a stress-controlled, gradient-based shape optimization process on a voxel mesh is targeted, providing the basis for integrating the enforcement of machine-learned characteristics into structural optimization processes.

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