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3D FEM modelling of geological structures caused by geometrical instabilities and contrasts in rock strength

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Many three-dimensional (3D) structures in rock, which formed during the deformation of the Earth's crust and lithosphere, are controlled by a difference in mechanical strength between rock units and are often the result of a geometrical instability. Such structures are, for example, folds, pinch-and-swell structures (due to necking) or cuspate-lobate structures (mullions). These structures occur from the centimeter to the kilometer scale and the related deformation processes control the formation of, for example, fold-and-thrust belts and extensional sedimentary basins or the deformation of the basement-cover interface. The 2D deformation processes causing these structures are relatively well studied, however, several processes during large-strain 3D deformation are still incompletely understood. One of these 3D processes is the lateral propagation of these structures, such as fold and cusp propagation in a direction orthogonal to the shortening direction or neck propagation in direction orthogonal to the extension direction. We study the 3D evolution of geometrical instabilities with numerical simulations based on the finite element method (FEM). Simulating geometrical instabilities caused by sharp variations of mechanical strength between rock units requires a numerical algorithm that can accurately resolve material interfaces for large differences in material properties (e.g. between limestone and shale) and for large deformations. Therefore, our FEM code combines a numerical contour-line technique and a deformable Lagrangian mesh with re-meshing. With this combined method it is possible to accurately follow the initial material contours with the FEM mesh and to accurately resolve the geometrical instabilities. The algorithm can simulate 3D deformation for a visco-elastoplastic rheology. Stresses are limited by a yield stress using a visco-plastic formulation and the viscous rheology is described by a power-law flow law. The 3D FEM code is applied to model 3D power-law folding and power-law Rayleigh-Taylor instabilities (diapirs) with different re-meshing scenarios. The results are tested with the analytical solution for small amplitudes and with 2D numerical results for large amplitudes. The code is further used to study the 3D lateral propagation of folding and viscoplastic necking from an initially localized perturbation and also the lateral propagation of cusps due to initial half graben geometry. Thereby, the small initial geometrical perturbations for folding and necking are exactly followed by the FEM mesh, whereas the initial large perturbation describing a half graben is defined by a contour line intersecting the finite elements, where more numerical integration points are applied in the corresponding elements. Furthermore, the code is applied to study 3D folding in an extensional setting.