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# A path-following simulation-based study of elastic instabilities in nearly-incompressible confined cylinders under tension



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# ABSTRACT

Recent experiments on hydrogels subjected to large elongations have shown elastic instabilities resulting in the formation of geometrically intricate fringe and fingering deformation patterns. In this paper, we present a robust numerical framework addressing the challenges that emerge in the simulation of this complex material response from the onset of instability to the post-bifurcation behavior. We observe that the numerical difficulties stem from the non-convexity of the strain energy density in the near-incompressible, largedeformation regime, which is responsible for the coexistence of multiple equilibrium paths with vastly-different, sinuous deformation patterns immediately after bifurcation. We show that these numerical challenges can be overcome by using sufficiently-high order of interpolation in the finite element approximation, an arc-length-based nonlinear solution procedure that follows the entire equilibrium path of the system, and an implementation enabling parallel, large-scale simulations. The resulting computational approach provides the ability to conduct highly-resolved, truly quasi-static simulations of complex elastic instabilities. We present numerical results illustrating the ability of the path-following approach to describe the full evolution of fringe and fingering instabilities observed experimentally in recent experiments of confined cylindrical specimens of soft hydrogels subject to tension. Importantly, we observe that the robustness of the static solution procedure enables complete access to the multiplicity of solutions occurring immediately after the onset of bifurcation, as well as to the settled post-bifurcation states.

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# 1. Introduction

Soft materials are commonly used in many technological applications. For example, they constitute parts of medical devices (Lind et al., 2017), deformable ionic conductors (Keplinger et al., 2013), and microfluidic devices (Domachuk et al., 2010). Owing to their ability to act as mechanical surrogates of tissues in the human body (*e.g.* muscles, tendons, or joints), soft materials are also widely employed in tissue engineering and regenerative medicine (El-Sherbiny and Yacoub, 2013;

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Lee and Mooney, 2001). Among the most promising materials in these applications are hydrogels, which constitute waterswollen networks of cross-linked polymer chains (Ahearne, 2014). As a result of the large water content and the relatively soft elastic behavior of the polymeric component, hydrogels have a large ratio of bulk and shear moduli (*i.e.* they are nearlyincompressible), and are therefore prone to develop elastic instabilities when subject to large deformations.

The study of mechanical instabilities in solids can be traced back to the buckling of structures with slender geometries, see for example (Bazant and Cedolin, 2010), and to the pioneering work of Biot (Biot, 1959), who studied the wrinkling of a free surface in elastomers subject to in-plane compression. In more recent times, a considerable body of literature has been concerned with the study of mechanical instabilities in solids, a complete review of which is beyond the scope of this paper. This work is a continuation of our recent experimental and theoretical study of mechanical instabilities arising in confined cylindrical specimens of soft hydrogels subject to large stretching (Lin et al., 2017). Specifically, we address the numerical challenges arising in the truly quasi-static simulation of the development and evolution of these mechanical instabilities. Previous related work includes (Biggins et al., 2013), where they reported the so called digital instability on a retreating meniscus at the boundary of an elastic layer under tension. This nonlinear deformation pattern has also been referred to as elastic fingering, due to its geometric similarity with the well-known Saffman-Taylor viscous fingering instability appearing at the interface between fluids of different viscosities (Saffman and Taylor, 1958). In contrast to viscous fingering, which is a dynamic process, elastic fingering occurs under quasi-static conditions (Biggins et al., 2013). Moreover, elastic fingering is fully reversible, rate-independent and enabled by the near incompressibility of the soft elastic layer (Biggins et al., 2013). It is also observed that, as the thickness of the layer is increased to a dimension comparable to or larger than the other dimensions, the instability localizes at the constrained fringes of the specimen, which has been appropriately referred to as fringe instability, (Lin et al., 2016). Similar instabilities have also been identified in cylindrical hydrogel specimens loaded in tension. In this case, the geometric patterns arising after the onset of the instability happen to be strongly dependent on the aspect ratio of the cylindrical samples (Lin et al., 2017) and on the strain-stiffening of the hydrogel (Lin et al., 2018). Interestingly, despite the geometric similarities between the fingering and fringe instabilities, they exhibit a qualitatively-different stressstretch response: monotonic in the case of fringe, and non-monotonic with a clear snap-through or potentially snap-back behavior in the case of fingering.

Extensive efforts have been focused on improving our understanding of these instabilities, which arise as bifurcations of equilibrium. Analytical techniques and numerical simulations have been developed to describe the evolution of the deformation under load, the onset of bifurcation, and the evolution of the post-bifurcated response characterized by the appearance of complex geometric patterns. In the specific case of the fringe instability in a constrained cylindrical hydrogel, the critical stress and stretch have been found analytically by Lin et al. (2016) by minimization of the elastic energy assuming an incompressible neoHookean material model. These results have been further developed by Lin et al. (2017), where the deformation patterns of instability have been obtained analytically with a linear perturbation analysis. Other analytical approaches recently employed to study mechanical instabilities include: nonlinear perturbation analysis, which has been applied to study wrinkle-to-fold transition (Ciarletta, 2014) and the elastic Rayleigh-Taylor instability (Chakrabarti et al., 2018); and singular perturbation analysis, which has been used in the study of crease nucleation (Ciarletta, 2018). These approaches have been very successful in describing basic features of the onset of the instabilities, but less so in the post-bifurcated regime. An instance of an analytically accessible post-bifurcation feature is the spatial wavelength of fringe and fingering deformation patterns. However, the amplitude of the fingers could not be obtained by analytical means (Lin et al., 2017). Similar limitations have also been found in the analytical study of other types of instabilities in solids. For example, the existence and the onset criterion of wrinkling instability modes emerging on the free surface of an elastic half space under compression were established in Biot (1959). In this case, however, mathematical models that can be treated analytically lack a characteristic length and, therefore, are unable to capture the wrinkle wavelength. Another relevant case is that of the formation of creases in an elastic half-space under compression, where an asymptotic approximation of the crease solution has been found (Ciarletta, 2018), although the analysis has not been able to resolve the indeterminacy of the crease radius and depth. It is then clear that the full post-bifurcation response of elastically-unstable solids is, in general, beyond analytical treatment.

It has been well-established that computational analysis can complement the analytical approach by providing a full description of the evolution of elastic instabilities far beyond the onset of bifurcation. However, the numerical simulation of the truly quasi-static evolution of elastic instabilities in general, and fringe and fingering in particular, presents significant difficulties. One of them is associated with attempting to describe the multiple equilibrium configurations near and beyond the bifurcation point, including the possibility of snap-back and snap-through. To avoid the issue, previous computational descriptions have treated the problem as dynamic, taking advantage of the robustness of explicit time integration schemes. However, as is well known, this approach introduces spurious inertia effects and imposes severe restrictions on the accessible time scales. These limitations can be mitigated to a certain extent by using techniques such as mass scaling (Lin et al., 2016), or more expensive implicit methods combined with numerical damping and adaptive time stepping (Biggins et al., 2013). Inertia effects may also preclude the description of non-monotonic effects such as snap-back. It is clear that, owing to the quasi-static nature of the problem, a more adequate solution approach would rather follow the equilibrium path of the system. However, it has recently been argued that the simulation of these elastic instabilities can only be performed after introducing artificial dynamics to the model. For example, in Biggins et al. (2013) the authors argue that, as a consequence of the sub-critical nature of the fingering bifurcation, transition to fingering cannot be simulated using equilibrium methods. Similar arguments have been presented in the case of creasing simulation, see supplemental information in Cao and Hutchinson (2012), where it is asserted that a pseudo-dynamic regularization of the problem is needed, as static nonlinear solvers would otherwise fail. However, static simulations have actually been proven viable in the context of a number of problems with similar numerical challenges including: formation and disappearance of crease (Chen et al., 2014; Ciarletta, 2018) and sulcification patterns (Hohlfeld and Mahadevan, 2012), and in the simulation of snap-through instabilities of pressurized balloons in Wang et al. (2018). In all these cases, the enabler was an adequate choice of the nonlinear solution method. Here, we show that the full evolution of fringe and fingering instabilities is accessible to quasi-static simulations, provided that a careful selection and orchestrated application of specialized algorithms is made. In fact, the difficulty in the static approach arises from several challenges that have been addressed and solved individually in the past and appear here in combination. Specifically, the numerical complexity stems from: 1) the near incompressibility, which on one hand implies the non-convexity of the saddle-point strain energy landscape (Ball, 1977) responsible for the bifurcation and the non-unique post-bifurcation response, while on the other hand may cause numerical locking as a result of a poor discretization; 2) the highly non-monotonic quasi-static large-deformation response, which requires specialized static nonlinear solvers; and 3) the sinuous deformation patterns, which demand a highly-resolved spatial description.

The aim of this work is to demonstrate the feasibility of the truly quasi-static path-following simulation of elastic instabilities in the specific context of the fringe and fingering experiments of cylindrical hydrogel specimens subject to large tensile stretching presented in Lin et al. (2017). We present a computational framework where all the ingredients are carefully chosen and adapted to address the numerical complexity of the problem. Specifically, the challenge of high-resolution of the instability patterns is addressed by adopting high-order finite element interpolations as well as a parallel computational framework based on domain decomposition suitable for large-scale simulation. Adopting high-order finite elements also overcomes the issue of numerical locking. To address the complexities associated with the non-monotonic highlynonlinear response at the onset and beyond the bifurcation point, we employ the arc-length method pioneered by Riks in Riks (1979) and then adapted for the use within the finite element method by Crisfield in Crisfield (1981a,b). The arc-length method has been successfully applied in the numerical simulation of quasi-static problems characterized by non-monotonic load-deformation curves in the past, including in the analysis of buckling of slender structures (Hill et al., 1989), crack propagation (Carpinteri and Monetto, 1999), and, more recently, in the study of elastic instabilities in Chen et al. (2014); Hohlfeld and Mahadevan (2012). The arc-length method enables the effective tracking of the quasi-static evolution of the problem without resorting to transient calculations affected by dynamic or inertia effects. An iterative algorithm to numerically solve the equations arising from the arc-length problem is implemented for multi-processor computation on distributed-memory systems, in which each processor contributes to the assembly and solution of the linearized problem in parallel. We apply the resulting computational framework to simulate fringe and fingering instabilities in cylindrical hydrogel samples under tension. We analyze in detail the transition to bifurcation and we show that a multiplicity of post-bifurcation equilibrium solutions exhibiting complex snap-through and snap-back response is accessible to the static numerical approach.

The present paper is structured as follows: Section 2 includes a detailed description of the morphology of the instability patterns observed experimentally and the main conclusions of an analytical study of fringe and fingering instabilities in cylindrical geometries. Section 3 describes the computational approach, including the high order finite element formulation, the arc-length nonlinear solver employed, and the details of the parallel computing strategy enabling high-performance simulations. Section 4 presents numerical experiments conducted to demonstrate the ability of the proposed computational framework to successfully deal with the severe numerical complexities discussed above in comparison with more traditional approaches. Convergence and robustness are also assessed in that section, in addition to verification against available analytical results for the pre-bifurcation regime. In Section 5 we present the results of the path-following simulations of fringe and fingering instabilities discussing the morphology of the deformation patterns and their evolution in the post-bifurcation regime. Conclusions are drawn in Section 6. Finally, Appendix A presents in detail the arc-length algorithm, which has been adapted to consider Dirichlet boundary conditions, as required by the simulations.

## 2. Summary of experimental and analytical results

As mentioned in the introduction, we use our recent experimental results on the unstable elastic response of soft elastic cylinders (Lin et al., 2017) as the main drivers for the development of the computational simulation framework. The interest in these specific experiments stems from the complex elastic response, which brings out the aforementioned numerical challenges, while providing a clear physical evidence of the specific deformation patterns that can be used as a basis for comparison with numerical predictions.

The specific experimental configuration consists of a cylindrical hydrogel specimen robustly bonded to glass substrates on its circular faces, as sketched in Fig. 1. The specimen is stretched by separating apart the attached ends in the longitudinal direction at a low strain rate  $\dot{e}_{exp} = 0.016 \, \text{s}^{-1}$ . Since the adhesion of the hydrogel to the glass is very strong, the two circular faces remain undeformed in their original plane throughout the deformation. Initially, the deformation proceeds in an ostensibly axisymmetric manner, where the main noticeable feature is the thinning of the central section of the cylinder due to the large Poisson effect, and the formation of a meniscus near the ends of the cylinder due to the radial constraint provided by the bonded glass, Figs. 2(a) and 3(a). At a critical stretch, the axial symmetry of the exposed surface of the meniscus is broken and the shape of the surface becomes unstable, evolving into sinuous geometric patterns resembling finger-like structures. Depending on the aspect ratio  $\alpha$  of the cylindrical sample, defined as the ratio between its diameter and height, two distinct geometric patterns have been observed (Lin et al., 2016). In the case of large aspect ratios



Fig. 1. A schematic of the experimental setup from Lin et al. (2017).



(a) pre-bifurcation

(b) post-bifurcation

**Fig. 2.** Snapshots of intermediate (a) and final (b) deformed configurations observed in the tensile tests of cylindrical hydrogel specimens with  $\alpha = 1$ . The figure on the left shows the radially-symmetric deformation pattern for a stretch  $\bar{\lambda} = 2$  which persists until the onset of bifurcation. The right figure shows the final deformed state for a stretch  $\bar{\lambda} = 4$  where the fringe instability can clearly be observed.

 $(6 \le \alpha \le 20)$ , i.e. very flat penny-shaped cylinders, deformation patterns resembling fingers encompassing the whole length of the sample arise at stretches of the order of  $\overline{\lambda} = 1.5$ , Fig. 3(b). This instability is known as *fingering*. In the case of low aspect ratios ( $\alpha \le 4$ ), *i. e.* taller cylinders, the fingers appear only next to the cylinder ends and for much larger stretches of the order of  $\overline{\lambda} = 5$ , Fig. 2(b). This instability is known as *fringe*. In the intermediate range ( $4 \le \lambda \le 6$ ), there is a transition between the two types of deformation structures.

An analytical solution to the problem of an incompressible neo-Hookean cylinder subject to large tensile stretches prior to the onset of the instability was also obtained in Lin et al. (2017). One of the main results of the analysis is that the stress-stretch response can be expressed as follows:

$$\frac{S}{\mu} = S_0(\kappa) + \alpha^2 S_1(\kappa), \tag{1}$$

where *S* is the nominal stress and  $\kappa$  is a loading parameter related to the stretch  $\overline{\lambda}$  through the following formula:

$$\bar{\lambda} = \frac{\sinh(2\kappa)}{2\kappa}.$$

In Eq. (1)  $S_0$  and  $S_1$  are non-dimensional functions of  $\kappa$  only whose detailed expressions can be found in Lin et al. (2017). An interesting observation about these quantities is that  $S_0$  is two orders of magnitude larger than  $S_1$  for a vast range of tensile stretches. As a consequence, aspect ratios of order 10 are necessary for  $S_1$  to contribute to the nominal stress in a significant way, whereas for lower values of  $\alpha$  the stress is dominated by  $S_0$ . Consistently with what is observed in the experiments, two different pre-bifurcation regimes can be identified depending on the aspect ratio of the sample, each giving rise to a different type of post-bifurcation response: fringe is observed for order-one values of the aspect ratio, whereas fingering appears for aspect ratios of order 10 and higher.

The analytical stress-stretch response of Eq. (1) was obtained in Lin et al. (2017) assuming axial symmetry and incompressibility, and is valid prior to the onset of fringe and fingering instabilities. The onset of bifurcation, in terms of the critical stretch, was also obtained in Lin et al. (2017) by a linear perturbation analysis of the axisymmetric deformation. In



**Fig. 3.** Snapshots of intermediate (a) and final (b) deformed configurations observed in the tensile tests of cylindrical hydrogel specimens with  $\alpha = 12$ . The figure on the left shows the radially-symmetric deformation pattern for a stretch  $\bar{\lambda} = 1.1$  which persists until the onset of bifurcation. The right figure shows the final deformed state for a stretch  $\bar{\lambda} = 1.5$  where the fingering instability can clearly be observed.



**Fig. 4.** Sketch of the reference configuration  $\Omega_0$ . The boundary of the domain is partitioned in the top face  $\Gamma_D$ , where an increasing imposed displacement is set, the lateral surface  $\Gamma_N$  with traction-free boundary conditions, and the symmetry section  $\Gamma_S$  with symmetry boundary conditions, i.e. vertical displacement fully constrained and free lateral displacements.

Section 4.5 we will use these analytical results to verify the numerical predictions of our computational framework prior to the onset of bifurcation.

## 3. Computational framework

The numerical description of the quasi-static formation of fingering and fringe instabilities requires a careful selection of discretization and solution algorithms, as a naive application of conventional well-established finite element methods fails to capture the relevant physics. In the following we present the details of our computational framework.

In the simulation of the deformation history of the cylindrical hydrogel specimens as the applied stretch is increased, the numerical challenge of locking arises immediately in the early linear regime. To prevent the well-known locking phenomenon, we employ high-order finite element interpolations, which also address the need for high resolution of the computational domain. While evolving towards the large deformation elastic regime, near incompressibility brings along two more challenges, in addition to numerical locking. In fact, even though locking is avoided via high-order finite elements, the jacobians arising in the linearized problem are still near-singular. We address the resulting ill-conditioning of the algebraic systems by taking advantage of the robustness of *direct* linear solvers, as opposed to *iterative* linear solvers. We remark that near incompressibility not only cause numerical difficulties, but also implies the non-convexity of the energy landscape (Ball, 1977), which is responsible for the bifurcation. We deal with the non-monotonic quasi-static response with a specialized *path-following* nonlinear solver, which robustly allows for the numerical tracking of the incremental equilibrium states without the pollution of artificial dynamic effects. Finally, the simulation of these complex inherently three-dimensional deformation patterns demands high-performance large-scale simulation capability.

In the spatial finite element discretization of the experiments described in 2, we consider as computational domain a cylinder with diameter *D* and height *H*, whose aspect ratio is  $\alpha = D/H$ . Fig. 4 shows a schematic of the computational domain with a description of the boundary conditions applied. The lateral surface  $\Gamma_N$  is assumed traction free. The top surface  $\Gamma_D$  is subject to an increasing imposed displacement  $\bar{u}$  in the axial direction and constrained from displacing laterally, which

assumes perfect adhesion of the material to the moving plate. Finally, exploiting the symmetry of the problem, we model half of the cylinder and impose symmetry boundary conditions on the mid-surface of the specimen  $\Gamma_s$ .

The discretized finite element formulation results in a nonlinear system of algebraic equations representing equilibrium of forces for all the nodal degrees of freedom of the domain discretization:

$$\boldsymbol{F}^{\text{int}}(\boldsymbol{u}) = \boldsymbol{F}^{\text{ext}}.$$

In (2),  $\mathbf{F}^{int}$  is the array of internal nodal forces,  $\mathbf{u}$  is the array of unknown nodal displacements resulting from the Galerkin approximation of the displacement field, and  $\mathbf{F}^{ext}$  is the array of external nodal forces resulting from the essential boundary conditions, as in our case we do not consider body forces or inhomogeneous Neumann boundary conditions. The internal forces depend nonlinearly on the discrete displacement field. More precisely, the force  $f_{ia}^{int}$  on degree of freedom *i* of discretization node *a* is given by

$$f_{ia}^{int}(\boldsymbol{u}) = \int_{\Omega_0} P_{il}(\boldsymbol{u}) N_{,l}^a \, \mathrm{d}V, \tag{3}$$

where  $P_{il}$  denotes the components of the first Piola-Kirchhoff stress tensor,  $N_I^a$  is the partial derivative of global shape function  $N^a$  with respect to coordinate  $X_I$  in the reference configuration. In the finite element discretization of the equilibrium Eq. (2) we employ specialized high-order interpolation spaces. Specifically, we adopt multivariate high-order polynomial functions with optimized distribution of nodal locations (Warburton, 2006), and we perform the integration in space in Eq. (3) employing the fully symmetric and positive quadrature rules proposed in Zhang et al. (2009). This combination of specialized interpolation functions and quadrature rules has been shown to minimize the ill-conditioning of the stiffness matrix among other alternatives.

We adopt a hyperelastic constitutive model of the compressible neoHookean type, with the following strain energy density potential:

$$W = \frac{\lambda}{2} (\log J)^2 - \mu \log J + \frac{\mu}{2} (tr(\mathbf{C}) - 3),$$
(4)

which allows us to explore the transition from compressible to nearly-incompressible response and its effect on the onset and development of fringe and fingering instabilities. In this expression,  $\lambda$  and  $\mu$  denote the infinitesimal Lamé parameters<sup>1</sup>, *J* is the determinant of the deformation gradient *F*, and  $C = F^T F$  is the right Cauchy-Green tensor. This constitutive model has also been adopted in similar studies, Cao and Hutchinson (2012); Ciarletta (2018); Lin et al. (2017). As is well known, Ball (1977), in the incompressible limit  $\frac{\mu}{\lambda} \rightarrow 0$ , the strain energy density *W* is necessarily non-convex, as the valleys must lie on the hyper surface satisfying the constraint  $\lambda_1 \lambda_2 \lambda_3 = 1$ , where  $\lambda_i$  are the principal stretches. In our case, it is instructive to express *W* in this way and explore its structure in the transition to incompressibility.

$$W(\lambda_1, \lambda_2, \lambda_3) = \frac{1}{2}\lambda \log^2 (\lambda_1 \lambda_2 \lambda_3) - \mu \log (\lambda_1 \lambda_2 \lambda_3) + \frac{1}{2}\mu \left(\frac{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}{(\lambda_1 \lambda_2 \lambda_3)^{2/3}} - 3\right)$$
(5)

Fig. 5 shows contours of the strain energy function (4) in principal stretch space  $\lambda_1$ ,  $\lambda_2$  for fixed  $\lambda_3 = \overline{\lambda} = 2$ . When  $\lambda \sim \mu$ , Fig. 5(a), the shape of the contours clearly show that the strain energy remains convex for a large range of deformations. By contrast, when  $\lambda \gg \mu$  and the material becomes more incompressible, Fig. 5(b), the contours adopt a "banana" shape which is indicative of the non-convexity of *W*. The main implication is that vastly-different local deformations can coexist with the same strain energy level, which explains the possibility of bifurcation and non-uniquess of the solution. As a specific example, it is clear from the figure that one would obtain the same energy level for a deformation with a given imposed value  $\lambda_3 = \overline{\lambda}$  with either small  $\lambda_1$  and large  $\lambda_2$  or vice versa.

The proper choice of an iterative solver for the nonlinear system of Eq. (2) is critical. Among the widest-used approaches for nonlinear problems in solid mechanics is the Newton-Raphson method, which can be driven either by applied forces or imposed displacements. However, if the system exhibits non-monotonic features in the equilibrium path, *e.g.* snap-through, Fig. 6 (left) or snap-back, Fig. 6 (right), this approach struggles to converge near the critical points and fails to capture intermediate equilibrium configurations (*i.e.* between A and B, and between C and D in Fig. 6). To address this problem we adopt the so-called *arc-length* method originally proposed by Riks (Riks, 1979) as a robust alternative to force control and displacement control to address the same limitations, see also Crisfield (1981a,b). The basic idea behind arc-length control is to find the next equilibrium state by a path-following approach, geometrically intersecting the path of the internal forces with a sphere-like surface in the force-displacement space, or *solutions* space, centered in the starting equilibrium configuration, Fig. 7. Conceptually, this guarantees the intersection of the driving force with all possible points in the equilibrium path with a suitable adjustment of the size of the sphere-like surface, therefore providing numerical robustness. The arc-length method has been successfully employed to numerically describe snap-through and snap-back in several problems characterized by non-monotonic load-deformation curves, including buckling analysis of slender structures (Hill et al., 1989), snap-back analysis of quasi-static fracture propagation (Carpinteri and Monetto, 1999), and, more recently, snap-through instabilities of pressurized balloons (Wang et al., 2018).

<sup>&</sup>lt;sup>1</sup> there should be no confusion with the principal stretches  $\lambda_i$ 







**Fig. 6.** Non-monotonic behaviors of the stress-stretch equilibrium paths: snap-through (left) and snap-back (right). A force-driven approach is not able to reproduce numerically the softening between the states A and B. Similarly, a displacement-driven approach is not able to obtain the equilibrium states between the states C and D.



**Fig. 7.** A sketch of displacement control, force control, and arc-length control, which drive the system with increments of  $\Delta u$ ,  $\Delta F$ , and  $\Delta l$ , respectively. The solid line represents the internal forces, whereas the three dashed lines represent the constraints of displacement control, force control and arc-length control.

We briefly summarize here the mathematical formulation of the arc-length method and leave the implementation details to Appendix A. The formulation of the arc-length control method starts by introducing the concept of a distance *d* between two states on the solutions space. This distance can be defined, for example, in terms of the distances  $\Delta u$  and  $\Delta F$  measured on the displacement and force axis respectively:

$$d^{2}(\Delta \boldsymbol{u}, \Delta \boldsymbol{F}) = \Delta \boldsymbol{u} \cdot \Delta \boldsymbol{u} + \psi^{2} \boldsymbol{K}_{0}^{-1} \Delta \boldsymbol{F} \cdot \boldsymbol{K}_{0}^{-1} \Delta \boldsymbol{F}.$$
(6)

In Eq. (6),  $\psi$  is a nondimensional parameter that defines the relative weight of displacement and force contributions to the distance, while  $\mathbf{K}_0$  is the initial Jacobian tensor, which plays the role of a scaling parameter. The isolines of function (6) identify ellipsoids in the solutions space, which may reduce in limiting cases to spheres ( $\psi = 1$ ) or cylinders ( $\psi = 0$ ), leading to arc-length formulations known as *spherical* and *cylindrical*, respectively.

The solution procedure to find the next equilibrium point involves setting a desired size  $\Delta l$  of the sphere-like surface, leading to the following scalar constraint equation:

$$d^2(\Delta \boldsymbol{u}, \Delta \boldsymbol{F}) = \Delta l^2.$$
<sup>(7)</sup>

Notice that in this equation both  $\Delta u$  and  $\Delta F$  are unknown, whereas  $\Delta l$  is a prescribed arc-length increment, which may be increased or decreased adaptively to obtain smaller or bigger load steps, and thus track any equilibrium path however intricate. Compared to the formulation in Crisfield (1981a), the only modification is that we have premultiplied the force increment with the inverse of the initial Jacobian tensor for the sake of dimensional consistency.

Under the assumption that the imposed force does not change direction between consecutive equilibrium configurations, it is possible to express  $\Delta F$  as  $q\Delta s$ , where the nondimensional scalar *s*, referred to as *load factor*, is unknown, and the vector



Fig. 8. Mesh of the computational domain with aspect ratio  $\alpha = 6$ . The characteristic length of the elements close to the boundary  $\Gamma_N$  is approximately ten times smaller than the size of the central elements. In this case, the smallest element has size  $h = 5 \cdot 10^{-5}$ m.

q is a unit load vector parallel to  $F^{ext}$ . The equilibrium equations are then modified as follows:

$$\boldsymbol{F}^{m}(\boldsymbol{u}_h) = \boldsymbol{s}\boldsymbol{q}. \tag{8}$$

The coupled Eqs. (7) and (8) can be solved with Newton-Raphson's method and determine, given  $\Delta l$ , the increment of displacement  $\Delta u$  and load factor  $\Delta s$  between consecutive load steps, identifying the next equilibrium on the solutions space. Several numerical aspects of the arc-length procedure and the details of its implementation, with special emphasis on the treatment of Dirichlet boundary conditions (*i.e.* imposed displacement) and on the iterative strategy employed to solve the nonlinear coupled problem (7) and (8) are included in Appendix A.

We have implemented the described computational framework in our research code Summit ( $\Sigma$ MIT, The  $\Sigma$ MIT Development Group (2018)), which is a finite element library suitable for large-scale simulations. Parallel scalability is achieved by partitioning the computational domain using a domain decomposition technique. Each processor is then responsible for assembling its own portion of the Jacobians and residuals resulting from the discretization. The parallel solution of the linearized system in each iteration is handed to the PETSc library (Balay et al., 2016), which provides robust implementations of a wide-range of direct and iterative linear solvers. Due to the ill-conditioning of the linearized systems resulting from near incompressibility, we have found that direct solvers furnish more robust results albeit less scalable. We therefore adopt the parallel direct solver MUMPS (Amestoy et al., 2001; 2006) based on a Gaussian LU factorization available through the PETSc library to solve all linear systems arising from the discretization.

#### 4. Numerical experiments and verification

We present the results of numerical simulations of fringe and fingering instabilities in nearly-incompressible elastic cylindrical samples obtained with the computational framework detailed in Section 3. We model the hydrogel material used in the experiments using a compressible neoHookean material model, Eq. (4), with a shear modulus  $\mu = 5 kPa$  (Lin et al., 2017). We increase Poisson's ratio  $\nu$  to approach the incompressible limit. As we will discuss in Section 4.2, we have found that adopting a Poisson's ratio  $\nu = 0.4975$ , which corresponds to  $\lambda = 1$  MPa, captures the instabilities of interest while preserving the well-posedness of the jacobians.

We investigate the different types of instability arising for several values of the aspect ratio  $\alpha$ , by maintaining the initial height *H* of the cylinder constant (*H* = 1 mm), while computing the diameter *D* for each specific aspect ratio as  $D = \alpha H$ . A sample mesh of the computational domain for  $\alpha = 6$  is shown in Fig. 8. The meshes employed are unstructured and consist of tetrahedral elements, with refinement near the circumference, where we expect the largest deformation gradients. There is no need to introduce additional imperfections to capture the instability modes as the mesh itself introduces imperfections in the numerical model as a natural breakdown of axial symmetry in the geometry and therefore all the differential and integral operators involved in the weak formulation of the problem. During the stable portion of the deformation leading up to the point of bifurcation this has an imperceptible effect on the results. At the bifurcation point, the accumulated errors (imperfect axisymmetric mesh geometry, propagated round-off errors incurred in linear solves, finite tolerance in nonlinear convergence criterion) are sufficient to trigger a specific instability mode. Clearly, the nucleation of a specific unstable deformation structure (e.g. the location of the lobes along the circumferential direction) is dependent on the initial mesh, just as it would be in the case of an externally applied imperfection.

As discussed in Section 3, we employ arc-length control to track the evolution of the instabilities from the undeformed state to their full development. The arc-length measure  $\Delta l$  plays the role of the load step size. As described in Appendix A,  $\Delta l$  is initially set by imposing a value of the load factor  $\delta s_{initial}$ , Eq. (A.16), and then adaptively modified throughout the computation to obtain smaller or bigger load steps. The initial value of the nondimensional load factor varies from  $\delta s_{initial} = 0.01$ , for higher aspect ratios, to  $\delta s_{initial} = 1$ , for lower aspect ratios. With reference to the notation of the appendix, we set in our tests the load direction choosing  $\bar{u} = (0, 0, \frac{1}{100} \frac{H}{2})$ . Finally, we set the numerical parameters of the arc-length solver to the following values:  $\psi = 1$  (spherical arc-length), M = 0.5,  $n_D = 3$ .

int



**Fig. 9.** Final configuration ( $\lambda = 3.7$ ) of a cylindrical sample with aspect ratio  $\alpha = 1$  for several values of the polynomial interpolation order *p*.



**Fig. 10.** Influence of Poisson's ratio on the simulated response. Stress-stretch curves (left) and deformed cross-sections at nondimensional height z = 0.85 for the final deformed state  $\overline{\lambda} = 4$  (right), for  $\nu = 0.3$  (blue),  $\nu = 0.4$  (orange),  $\nu = 0.49$  (green), and  $\nu = 0.4975$  (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

### 4.1. Influence of p-refinement on simulated deformation patterns

As described above, the proposed strategy to avoid numerical locking due to incompressibility and at the same time to spatially resolve the intricate deformation patterns arising post instability, is to employ finite element interpolation of increasing polynomial order p. In the following, we investigate the influence of increasing p (p-refinement) on the ability to numerically capture the formation of fringe instabilities. We simulate the stretching up to  $\bar{\lambda} = 3.7$  of a cylindrical sample of aspect ratio  $\alpha = 1$  with four different values of  $p = 1, \ldots, 4$ , while coarsening the mesh to keep constant the total number of nodal degrees of freedom (approximately 240000). The fringe undulation is hardly visible if linear elements are used, while the axisymmetry is slightly broken when employing quadratic finite elements, Fig. 9. The fringe instability is instead well-developed in case of finite elements of order p = 3, whereas p = 4 does not seem to provide any higher resolution of the deformation patterns. For this reason, we adopt p = 3 for all subsequent investigations.

## 4.2. Influence of Poisson's ratio on simulated deformation patterns

Fringe and fingering instabilities arise as bifurcations in a system governed by a non-convex saddle-point energy landscape, which results from material near incompressibility. To investigate the influence of Poisson's ratio on the formation of the undulation patterns characterizing these elastic instabilities, we perform a series of simulations of a cylindrical sample of aspect ratio  $\alpha = 1$  with several values of Poisson's ratio,  $\nu = 0.3, 0.4, 0.49, 0.4975$ . Fig. 10 shows the simulated stress-stretch



**Fig. 11.** (a) Comparison of displacement control and arc-length control based nonlinear solvers. The solver based on traditional displacement control fails to converge in the simulation of fingering instability ( $\alpha = 5$ ). (b) A zoom in the neighborhood of the onset of bifurcation shows a snap-back in the equilibrium path for fingering instability.

curves and the deformation patterns at a cross-section close to the fringe for a stretch  $\overline{\lambda} = 4$ . These results clearly show that, even though the stress-stretch curves for  $\nu = 0.49$  and  $\nu = 0.4975$  almost overlap, the undulating deformation patterns only emerge for  $\nu = 0.4975$  or higher. However, to preserve the well-posedness of the jacobians, we adopt  $\nu = 0.4975$  for the remainder of the paper.

#### 4.3. Comparison of arc-length control with traditional load-control

As discussed in Section 3, nonlinear solvers based on displacement or force control are not able to capture all equilibrium states in problems characterized by a non-monotonic stress-stretch response. In some cases, see for example (Ciarletta, 2018), a priori knowledge of some features of the equilibrium curve (e.g. the critical load and the qualitative response after the critical load) can help tailor a successful strategy to obtain post-bifurcation equilibrium states. However, when this information is not accessible beforehand, neither approach is able to follow general non-monotonic equilibrium responses.

In this section we compare the numerical results obtained for a specimen of aspect ratio  $\alpha = 5$ , which exhibits fingering instability, with two different approaches: displacement control and arc-length control. Fig. 11(a) shows that displacement control is not able to reproduce numerically the post-bifurcation equilibrium states of fingering instability. More precisely, we observe that the nonlinear iterations of the solver based on displacement control fail to converge at some critical stretch (state A), where the stress-stretch curve presents a snap-back, Fig. 11(b). Beyond state A, traditional displacement control may directly 'snap' to state B, skipping all intermediate equilibrium states. However, due to the ill-conditioning of the stiffness matrix, the traditional displacement control solution procedure is not able to perform the snap, but rather fails to reach convergence.

Importantly, we remark that both displacement control and arc-length control are able to drive the system through the initiation and post-bifurcation of fringe instability, which develops without loss of monotonicity in the stress-stretch response.

## 4.4. Comparison against explicit dynamics simulations

The appeal and popularity of explicit time integration algorithms lies on their simplicity, expected numerical robustness and wide availability in commercial codes. The purpose of this section is to briefly expose the issues that emerge when trying to use this type of approach in the specific context of simulating the quasi-static formation of elastic instabilities.

To this end, we conducted simulations using the explicit Newmark method (Hughes, 2000) for a specimen with aspect ratio  $\alpha = 6$ . The static simulation took 27 h, most of which (about 90%) is spent in the post-bifurcation stage. A graded fine mesh of interpolation order p = 3 with characteristic element size h = H/8, where H = 1mm is the specimen height was used. This resulted in a mesh with 560K degrees of freedom. Attempts to run the explicit simulations with a coarser mesh led to premature termination of the simulation prior to the onset of instability due to severe mesh distortion and the vanishing of the stable time step. A lower bound to the number of explicit time integration steps required for given values of the final axial stretch  $\lambda_{fi}$  strain rate  $\dot{\varepsilon} = \nu/H$ , material longitudinal wave-speed  $c_L$  and characteristic mesh size h, can be



**Fig. 12.** (a) Stress-strain curves obtained for the case of fingering  $\alpha = 6$  using explicit dynamic simulations and different imposed strain rates. Comparison with static simulations. (b) Zoomed view near the bifurcation point.

estimated with the expression:

$$n \sim \frac{1}{\gamma} \frac{c_L}{\varepsilon h} (\lambda_f - 1), \tag{9}$$

where  $0 < \gamma \le 1$  is the CFL stability factor, and v is the imposed boundary velocity. For our specific case, the values:  $\lambda_f = 1.8$  (required to reach the post-bifurcation stage for this particular case of fingering), the experimental quasi-static strain rate  $\dot{\varepsilon}_{exp} = 0.016 \text{ s}^{-1}$ ,  $c_L = 31 \text{ ms}^{-1}$ , and  $\gamma = 0.9$ , result in  $n \sim 35$  million. In practice, the number of required time steps will be much higher because the stable time step decreases as the mesh distorts. For example, at the deformation levels expected when the lobes are formed, h could be many times smaller than in the undeformed configuration and the number of time steps will increase accordingly. The situation gets worse as the wave celerity increases when approaching the incompressible limit. It is then clear that running the explicit simulations under the real experimental quasi-static strain rate is in practice prohibitive. In order to obtain results in a reasonable amount of time, we conducted simulations with three different artificially-high strain rates of values  $10^r \times \dot{\varepsilon}_{exp}$  with r = 2, 3, 4, in order to explore a balance between computational time and deleterious artificial dynamic effects. The results are shown in Figs. 12 and 13. The following observations can be made:

- (r = 4, 10, 000 ×  $\dot{\varepsilon}_{exp}$ ) The response curve exhibits oscillations of the same order of magnitude of the stresses, Fig. 12(a), the simulation misses the bifurcation point and axisymmetry never breaks. The post-bifurcation instability patterns are not captured, Fig. 13(a). This simulation reaches  $\lambda_f = 1.93$  in 179000 time steps for a total computation time of T = 2.1 h. However, it is clear that it does not provide satisfactory results.
- (r = 3, 1000 ×  $\dot{\varepsilon}_{exp}$ ) The response curve exhibits oscillations of a smaller magnitude than the stresses but they are still noticeable, Fig. 12(b). In addition, the response curve misses the instability point. Neither softening nor snap-back are observed. Fig. 13(b) shows that the post-bifurcation patterns are not captured either at that stretch. This simulation reaches  $\lambda_f = 1.77$  in 1.25*M* time steps for a total computation time of T = 15.6 h. At that point, incipient formation of deformation structures is observed.
- $(r = 2, 100 \times \dot{\varepsilon}_{exp})$  The oscillations in the stress-stretch response are hardly noticeable, Fig. 12(b). In addition, the response curve overshoots the instability point. Softening is observed but snap-back is not. The post-bifurcation instability pattern with the same number of fingers emerges in a single configuration which evolves robustly with further stretch, Fig. 13(c). This simulation reaches  $\lambda_f = 1.71$  in 10.65*M* time steps for a total computation time of *T* = 123.5 h.

We observe that in order to capture the elastic instabilities, the explicit dynamics simulation will in general be much more expensive than the static counterpart. This can be alleviated by using artificial viscosity and mass-scaling techniques. However, the explicit simulations still miss the complex post-bifurcation response where the unstable deformation patterns can reconfigure through a series of snap-backs and snap-throughs until they settle into a final configuration. The static simulation provides full access to the post-bifurcation response in a much shorter computational time than the explicit dynamic simulations.

## 4.5. Verification of pre-bifurcation response

In this section we perform a verification of our computational approach against the analytical solution obtained in Lin et al. (2017) and discussed in Section 2. Fig. 14 shows a comparison of the stress-stretch response predicted by the





theory against our simulation results. We observe that the agreement is excellent before the onset of instability, beyond which the analytical solution is no longer valid.

The extended linear perturbation analysis performed in Lin et al. (2017) also provides a theoretical prediction of the critical stretch, which we have compared against the numerical prediction in Fig. 15. We identified the critical imposed stretch at which axisymmetry breaks in the simulations with the value  $\bar{\lambda}_c^n$  at which a sudden increase in the nonlinear shear strain  $\varepsilon_{r\theta}$  is observed at the free boundary.

## 4.6. Strong scaling and parallel performance

The parallel performance of our computational framework has been assessed via a strong scaling test performed on a cluster consisting of 30 nodes, each node having 24 Intel 2.3 GHz Xeon E5-2670 64-bit processors with 62.8 GB memory. Fig. 16 shows the wall time required to perform one converged load step, which consists of several nonlinear subiterations, for three different problem sizes (80000, 200000 and 450000 degrees of freedom) and for a number of processor ranging from 2 to 512.

The plot of Fig. 16 shows that in the proposed framework parallel computations can lead to significant reductions in the simulation time, *e.g.* the computation time per load step can be reduced from 1000 s to 100 s by employing 64 processors instead of 2 for a problem size of 200000 degrees of freedom. This also shows that the scalability is far from ideal, which can be attributed to well-known inefficiencies in parallel direct linear solvers (Saad, 2003). Better scalability could be obtained by employing parallel iterative linear solvers. However, the ill-conditioning of the jacobians in the presence of incompressibility brings about additional challenges requiring specialized preconditioners, which we have not pursued at this point.



Fig. 14. Comparison of normalized stress-stretch response from simulations and theory, Eq. (1), for selected values of the cylindrical specimen aspect ratio  $\alpha$ .



**Fig. 15.** Verification of the critical stretch  $\bar{\lambda}_c$  for bifurcation for several aspect ratios  $\alpha$ . The theoretical prediction  $\bar{\lambda}_c^t$  is taken from Lin et al. (2017), whereas  $\bar{\lambda}_c^n$  is the critical stretch evaluated numerically.



Fig. 16. Strong scaling test of a converged load iteration, consisting of several nonlinear iterations, for three different problem sizes, in terms of number of degrees of freedom (DOFs) of the discretization.



**Fig. 17.** Morphology of fringe instability. A cylindrical specimen with aspect ratio  $\alpha = 1$  is stretched to  $\overline{\lambda} = 4$ . On the right, slices of the sample orthogonal to the symmetry axis of the cylinder at several normalized heights z.

## 5. Analysis of fingering and fringe instabilities

In the following we apply the verified robust computational framework presented above to the investigation of fringe and fingering instabilities.

We first show that this approach is able to capture both fringe and fingering, as well as coexistence of the two instabilities, depending on the aspect ratio  $\alpha$  of the sample. Fig. 17 shows a hydrogel specimen with aspect ratio  $\alpha = 1$  subjected to an imposed stretch  $\overline{\lambda} = 4$ . On the right side of the picture we show four horizontal slices taken at different heights clearly indicating that the strongest oscillations of the free surface appear close to the specimen's fringes and far from the symme-





**Fig. 18.** Morphology of fingering instabilities. A cylinder with aspect ratio  $\alpha = 6$  is stretched up to  $\overline{\lambda} = 1.82$ . On the right, slices of the sample orthogonal to the symmetry axis of the cylinder at several normalized heights z.



**Fig. 19.** Combined fringe-fingering instabilities. A cylinder with a moderate aspect ratio,  $\alpha = 3$ , is stretched up to  $\overline{\lambda} = 3$ . On the right, slices of the sample orthogonal to the symmetry axis of the cylinder at several normalized heights *z*.

try plane. Notice that the boundary conditions do not allow the top face of the specimen to deform in its original plane, which causes the instability to disappear at the fringe wall.

Fig. 18 shows the results obtained by stretching a cylindrical specimen of aspect ratio  $\alpha = 6$  up to  $\overline{\lambda} = 1.82$ , exhibiting a typical morphology of fingering instability. In contrast to the previous case, the strongest oscillations occur at the symmetry plane z = 0 and gradually fade as the distance from the symmetry plane increases, as can be observed in the horizontal slices on the right side of the picture. Finally, we observe coexistence of fringe and fingering instabilities on a specimen of intermediate aspect ratio  $\alpha = 3$  stretched to  $\overline{\lambda} = 3$ , Fig. 19. The slices on the right clearly show that the undulations are strong at the symmetry plane (z = 0), as well as close to the specimen's fringes.

It is then interesting to investigate how the instabilities quasi-statically evolve from their first initiation to the fully developed deformation pattern. Fig. 20 shows 5 views at z = 0.9 of the deformed cylinder for  $\alpha = 1$  (fringe instability) at



**Fig. 20.** Fringe undulation for aspect ratio  $\alpha = 1$ . Top: Deformed configurations corresponding to several equilibrium states (view from a section of the cylinder close to the fringe, with normalized height z = 0.9). Each state is labeled with a number that corresponds to a point in the stress-stretch curve. Bottom: Stress-stretch equilibrium path.

different values of  $\overline{\lambda}$  and the corresponding equilibrium states on the stress-stretch curve. We observe that the response is monotonic and that the instability emerges near  $\overline{\lambda} = 3.5$ , State (3). The instability pattern adopts a shape with 9 lobes. All lobes emerge simultaneously and deepen in magnitude in a monotonic fashion as the load further increases, States (4) and (5).

Fig. 21 shows 8 views at z = 0 of the deformed cylinder for  $\alpha = 6$  (fingering instability) at different values of  $\overline{\lambda}$  and the corresponding equilibrium states on the stress-stretch curve. We observe that the response is qualitatively similar to that observed for fringe instability up to the critical point, exhibiting a monotonic increase of stress with the imposed stretch, while preserving an axisymmetric deformation pattern. Beyond the critical point the stress-stretch response differs substantially. Specifically, the lobes do not arise in a simultaneous fashion and leave part of the sample axisymmetric. Beyond State (3)





(7)  $\bar{\lambda} = 1.7135$ 

(1)  $\bar{\lambda} = 1.4067$ 

(8)  $\overline{\lambda} = 1.7849$ 



**Fig. 21.** Fingering undulation for aspect ratio  $\alpha = 6$  obtained with interpolation order p = 2. Top: Deformed configurations corresponding to several equilibrium states (view from the symmetry plane of the cylindrical sample). Each state is labeled with a number that corresponds to a point in the stress-stretch curve. Bottom-Left: Stress-stretch equilibrium path. Bottom-Right: Zoom in the neighborhood of the onset of bifurcation.

the stress-stretch exhibits a snap-back with a minimum  $\overline{\lambda}$  at State (4), where however the lobes are deeper. It is noteworthy that the arc-length procedure is able to track a branch of the equilibrium path where both stress and stretch decrease in a numerically robust fashion. The next equilibrium path between States (4) and (5), exhibits a softening response with an increase of stretch and a decrease of stress, a further deepening of the lobes and the emergence of new ones. Between States (5) and (6) another significant snap-back is observed which is characterized by drastic changes in the deformation, with the appearance of new lobes in different parts of the sample and disappearance of previously developed lobes. The equilibrium path exhibits a fairly erratic response between States (5) and (6) with large variations in the deformation patterns, which for

the sake of conciseness we do not show, and closely coexisting equilibrium states. Beyond State (6) the additional evolution of the stress-stretch curve shows a clear softening response up to a stretch of about  $\bar{\lambda} = 1.8$ . In this part of the equilibrium path the deformation pattern stabilizes and settles to a well defined set of lobes of equal increasing depth, States (7) and (8). The instability pattern adopts a shape with 7 lobes, matching the theoretical prediction for a specimen with aspect ratio  $\alpha = 6$ , (Lin et al., 2017). We observe that the main deformation mechanism during the softening portions of the response curve is the deepening of existing deformation structures, whereas in the snap-back portions is where the main deformation structures form or change into a new shape. This can be seen more clearly in the animations accompanying this paper in the supplementary material.

Given the complex non-monotonic response observed, with multiple vastly different deformation patterns seemingly coexisting within a small range of applied stretches and with very small differences in stress, the question arises of whether the order of accuracy of the simulations influences the results in a significant manner. The results shown in Fig. 21 have been obtained with a polynomial order of interpolation p = 2. Fig. 22 shows, instead, the results obtained with p = 3. The general observations still apply, including the predicted stress and stretch at the critical point and the predicted number of lobes, although a much richer and complex set of non-uniform and non-periodic deformation patterns is obtained. It is also confirmed that the formation of new deformation structures (States 3–4, 5–6, 6–7, and 7–8) coincides with portions of the stress-stretch curves dominated by significant snap-back, whereas during the softening portions of the response curve that do not exhibit snap-back (States 4–5, 8–9) existing structures evolve into a more pronounced state of deformation, see also the animations accompanying this paper in the supplementary material.

#### 6. Summary and conclusions

We presented a computational framework for conducting simulations of the onset and quasi-static evolution of elastic instabilities in soft nearly-incompressible materials subject to large deformations. The problem is particularly challenging from the numerical standpoint due to the incompressible nonlinear material response, which exhibits a highly non-convex energy landscape, leading to extremely interesting unstable deformation patterns which can coexist due to the non-uniquess of the solution.

We show that a *sine qua non* requirement for obtaining results that capture this complex response is the ability to: 1) treat the incompressibility constraint in a satisfactory manner, 2) resolve the strong gradients with enough accuracy, and 3) employ an adequate non-linear solution approach with the ability to follow intricate equilibrium paths. We accomplish these objectives by adopting a scalable approach based on high-order finite-element interpolation, an arc-length controlled nonlinear iteration procedure, and a linear solver behaving robustly in the presence of near incompressibility. In particular, we found that low order interpolation (p = 1, 2) fails to capture the relevant physics, whereas p = 3 and higher gives excellent characterizations of the experimentally-observed deformation patterns.

We also attempted to conduct simulations using explicit time integration. We found that running the explicit simulations under the real experimental quasi-static strain rates is computationally prohibitive. If the applied strain rate is thousands of times higher than in reality, reasonable computational times are obtained, but the numerical results are marred with dynamics oscillations which result in the inability to capture the elastic instability patterns. For a strain rate one hundred times higher than the experimental value, the deformation patterns are captured. In this case, the dynamic solution finds one of the possible paths and deformation pattern configurations beyond the bifurcation point and continuous to evolve in the post-bifurcation stage along the same path with a stable deformation pattern. The fundamentally greedy nature of the explicit time integration algorithm precludes the possibility of describing the multiplicity of solutions that arise beyond the bifurcation point with potentially-tortuous response paths (snap-through, snap-back). We conclude that the proposed quasi-static path-following approach is advantageous both in terms of capturing the post-bifurcation response as well as in its computational cost. We also found that static simulations are more robust with respect to initial mesh quality and deformation-induced mesh distortion, which gives access to the solution significantly past the bifurcation point.

We applied the framework to simulate the elastic response of cylindrical hydrogel specimens, which under very large tensile stretches develop instabilities of the fringe and fingering type. We verified the results where possible, i.e.: in the prebifurcation stage where an analytical solution of the stress-stretch response exists, and at the onset of bifurcation where a perturbation analysis gives the critical stretch and the number of lobes of the instability pattern. The parallel implementation enabling large-scale simulations with the required high resolution is shown to scale and provide significant computational speedup to the scalability limit of the direct linear solvers employed. Further scalability could be obtained by exploring the use of iterative solvers endowed with preconditioning schemes suitable for nearly-incompressible problems. But this has not been necessary and therefore has not been pursued at this point.

The simulation results unveiled a number of important characteristics of the post-bifurcation response. In the case of fringe (tall cylinders), the stress-stretch response remains monotonic throughout the bifurcation and post-bifurcation stages, and the deformation pattern that emerges at the bifurcation point is periodic around the circumference (i.e. all lobes arise simultaneously and have the same depth), and grows uniformly with the axial stretch.

By contrast, the case of fingering (flat cylinders) exhibits a much more complex response. Multiple equilibrium states where axisymmetric regions coexist with others that are non-axisymmetric are observed immediately after the bifurcation point. This coincides with a stress-stretch response characterized by a multiplicity of non-monotonic features including snap-throughs and snap-backs. It is found that the formation of new deformation structures coincides with portions of the





**Fig. 22.** Fingering undulation for aspect ratio  $\alpha = 6$  obtained with interpolation order p = 3. Top: Deformed configurations corresponding to several equilibrium states (view from the symmetry plane of the cylindrical sample). Each state is labeled with a number that corresponds to a point in the stress-stretch curve. Bottom-Left: Stress-stretch equilibrium path. Bottom-Right: Zoom in the neighborhood of the onset of bifurcation.

stress-stretch curves dominated by significant snap-back, whereas existing structures evolve into a more pronounced state of deformation during the softening portions of the response curve. Eventually, the response settles into a well-defined deformation pattern that grows in intensity in a uniform manner, similarly to the case of fringe.

It is a remarkable feature of the proposed path-following nonlinear iteration scheme that it can describe such complex deformation response in such a robust numerical manner. More specifically, the simulations not only captured the well-known and previously reported snap-through response (Lin et al., 2016), but also unveiled the significant presence of snap-backs in the stress-stretch response which are inaccessible to experiments and other numerical schemes due to the limitations imposed by displacement or load control.

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# Appendix A. Implementation details of the arc-length procedure

For the reader's convenience we report in this section all implementation details of the arc-length method. The coupled nonlinear problem described in Section 3, whose governing equations are:

$$\boldsymbol{F}^{int}(\boldsymbol{u}_h) = \boldsymbol{s}\boldsymbol{q},\tag{A.1}$$

$$\Delta \boldsymbol{u} \cdot \Delta \boldsymbol{u} + \boldsymbol{\psi}^2 \boldsymbol{K}_0^{-1} \boldsymbol{q} \cdot \boldsymbol{K}_0^{-1} \boldsymbol{q} \Delta \boldsymbol{s}^2 = \Delta l^2, \tag{A.2}$$

can be solved with an iterative process  $\hat{a}$  la Newton-Raphson. Let k denote the number of the arc-length iteration, also referred to as *nonlinear iteration*, to distinguish it from the *load iteration*, and  $\boldsymbol{u}_k$  and  $s_k$  the displacement and load factor of the current nonlinear iteration. We obtain the updated unknown displacement field and load factor as  $\boldsymbol{u}_{k+1}$  and  $s_{k+1}$  that satisfy the linearized force balance Eq. (A.3) and the arc-length Eq. (A.4):

$$F^{int}(u_k) + K(u_k)(u_{k+1} - u_k) = s_{k+1}q,$$
(A.3)

$$\Delta \boldsymbol{u}_{k+1} \cdot \Delta \boldsymbol{u}_{k+1} + \psi^2 \eta^2 \Delta s_{k+1}^2 = \Delta l^2, \tag{A.4}$$

where we set  $\eta^2 = ||\mathbf{K}_0^{-1}\mathbf{q}||^2$  to simplify notation. We recall that in (A.4),  $\Delta u_{k+1}$  and  $\Delta s_{k+1}$  are increments of the updated displacement field and load factor with respect to the previous known equilibrium state ( $\mathbf{u}^n$ ,  $s^n$ ), that is the solution at the previous load step, and that the arc-length nonlinear constraint represents in the load-displacement space a sphere, or in general an ellipsoid, centered in ( $\mathbf{u}^n$ ,  $\mathbf{F}^{int}(\mathbf{u}^n) = s^n \mathbf{q}$ ). Notice that we do not linearize Eq. (A.4). In this section we assume that the load vector  $\mathbf{q}$  is constant throughout all the arc-length procedure.

We define the increments of displacement and load factor between consecutive nonlinear iterations as follows:

$$\delta \mathbf{u}_{k+1} = \mathbf{u}_{k+1} - \mathbf{u}_k, \quad \delta s_{k+1} = s_{k+1} - s_k, \tag{A.5}$$

so that we can write the new increments  $\Delta u_{k+1}$  and  $\Delta s_{k+1}$  of displacement and load factor between consecutive load iterations, in terms of the previous  $\Delta u_k$  and  $\Delta s_k$ , as follows:

$$\Delta \boldsymbol{u}_{k+1} = \Delta \boldsymbol{u}_k + \delta \boldsymbol{u}_{k+1}, \qquad \Delta s_{k+1} = \Delta s_k + \delta s_{k+1}. \tag{A.6}$$

With this notation, Eq. (A.3) can be rewritten as:

$$\boldsymbol{K}(\boldsymbol{u}_k)\delta\boldsymbol{u}_{k+1} = \delta \boldsymbol{s}_{k+1}\boldsymbol{q} - \boldsymbol{R}_k, \qquad \boldsymbol{R}_k = \boldsymbol{F}^{int}(\boldsymbol{u}_k) - \boldsymbol{s}_k\boldsymbol{q}, \tag{A.7}$$

and the arc-length constraint (A.4) can be rewritten in the form:

$$||\delta \boldsymbol{u}_{k+1} + \Delta \boldsymbol{u}_k||^2 + \psi^2 \eta^2 (\delta s_{k+1} + \Delta s_k)^2 = \Delta l^2.$$
(A.8)

Given  $\boldsymbol{u}_k$  and  $s_k$ , one can solve Eqs. (A.7) and (A.8) for  $\delta \boldsymbol{u}_{k+1}$  and  $\delta s_{k+1}$  to advance from the state ( $\boldsymbol{u}_k$ ,  $s_k$ ) to the state ( $\boldsymbol{u}_{k+1}$ ,  $s_{k+1}$ ). Notice that the state ( $\boldsymbol{u}_{k+1}$ ,  $s_{k+1}$ ) is equilibrated only at convergence, as better detailed in the following.

To solve the system of Eqs. (A.7) and (A.8) we follow Crisfield's approach (Crisfield, 1981a). Specifically, we compute

$$\delta \boldsymbol{u}_{k+1} = \delta \boldsymbol{s}_{k+1} \boldsymbol{u}_{\boldsymbol{q},k} + \delta \boldsymbol{u}_{\boldsymbol{R},k},\tag{A.9}$$

where  $u_{a,k}$  and  $\delta u_{R,k}$  are the solutions of the following linear systems, respectively:

$$K(\boldsymbol{u}_k)\boldsymbol{u}_{\boldsymbol{q},k} = \boldsymbol{q}, \qquad K(\boldsymbol{u}_k)\delta\boldsymbol{u}_{\boldsymbol{R},k} = -\boldsymbol{R}_k, \tag{A.10}$$

and  $\delta s_{k+1}$  is obtained by solving the following second order scalar equation equivalent to (A.8):

$$a (\delta s_{k+1})^2 + 2b \,\delta s_{k+1} + c = 0, \tag{A.11}$$

in which the coefficients are computed using the available data from the k-th nonlinear iteration, i.e.

$$a := \psi^2 \eta^2 + ||\mathbf{u}_{\mathbf{q},k}||^2,$$
  

$$b := \psi^2 \eta^2 \Delta s_k + \mathbf{u}_{\mathbf{q},k} \cdot \delta \mathbf{u}_{\mathbf{R},k} + \mathbf{u}_{\mathbf{q},k} \cdot \Delta \mathbf{u}_k,$$
  

$$c := \psi^2 \eta^2 (\Delta s_k)^2 + ||\delta \mathbf{u}_{\mathbf{R},k}||^2 + 2\delta \mathbf{u}_{\mathbf{R},k} \cdot \Delta \mathbf{u}_k + ||\Delta \mathbf{u}_k||^2 - \Delta l^2.$$
(A.12)



**Fig. A1.** A sketch of the iterative process to solve the coupled arc-length problem. The superscript *n* is used to denote the known converged solution at the previous load step. The converged solution pair  $(u^n, s^n)$  and the parameter  $\Delta l$  identify the arc-length nonlinear constraint (*i.e.* the circumference in the plot). Given  $u_k$ , the state  $(u_{k+1}, s_{k+1})$  is obtained by intersecting the arc-length constraint with the linearization of the internal forces at  $u_k$ . Upon convergence, this procedure identifies the new equilibrium state  $(u^{n+1}, s^{n+1})$ . Note that  $F^{int}(u^n) = s^n q$  as well as  $F^{int}(u^{n+1}) = s^{n+1}q$ . This is clearly not the case for the intermediate predictions  $(u_k, s_k)$ , which are not equilibrated states in general.

This iterative procedure is sketched in Fig. A.23. The initialization and stopping criterion for this procedure will be discussed later on.

The treatment of Dirichlet boundary conditions as the driving load of the arc-length formulation is possible, even though it requires some care. Indeed, although the Dirichlet boundary conditions can be seen as Neumann boundary conditions where the force is the external force  $q_D$  necessary to constrain to  $\bar{u}$  the displacement on the Dirichlet portion  $\Gamma_D$  of the boundary, generalizing the arc-length formulation to this kind of external load is not straightforward for the following reasons:

- The algebraic systems to be solved in Eq. (A.10) are the *condensed* system of the equation involving the non-constrained  $N_N$  degrees of freedom, being N the total number of degrees of freedom, and  $N_D = N N_N$  the number of the constrained degrees of freedom. Each of these algebraic systems is to be solved with the appropriate imposed displacement.
- One cannot assume that the direction of the external load  $q_D$  is constant throughout the arc-length procedure, as it is the case for problems with Neumann boundary conditions. Indeed, one has  $q_D = -K_D(u)\bar{u}$ , where with  $K_D$  we mean the  $N_N \times N_D$  rectangular portion of the stiffness matrix involving the interaction between the  $N_D$  constrained degrees of freedom and the  $N_N$  free degrees of freedom.

To derive the proper arc-length formulation in case of Dirichlet boundary conditions, let us consider the following problem:

$$F^{int}(\boldsymbol{u}) = \boldsymbol{0},$$
  
subject to  $\boldsymbol{u} = s\boldsymbol{\bar{u}}$  on  $\Gamma_D$ , (A.13)

which can be linearized in the neighborhood of the state ( $\boldsymbol{u}_k, s_k$ ), giving rise to

$$\begin{aligned} \mathbf{F}^{int}(\mathbf{u}_k) + \mathbf{K}(\mathbf{u}_k) \,\,\delta \mathbf{u}_{k+1} &= \mathbf{0}, \\ \delta \mathbf{u}_{k+1} &= \delta s_{k+1} \bar{\mathbf{u}} \,\,\mathrm{on} \,\,\Gamma_D. \end{aligned}$$
(A.14)

After breaking the stiffness **K** into the free and the constrained sets of degrees of freedom and eliminating the equations for the imposed degrees of freedom, the condensed system of equations reads:

$$\boldsymbol{K}_{N}(\boldsymbol{u}_{k}) \ \delta \boldsymbol{u}_{k+1} = \delta \boldsymbol{s}_{k+1} \boldsymbol{q}_{D,k} - \boldsymbol{F}^{int}(\boldsymbol{u}_{k}), \tag{A.15}$$

where  $\boldsymbol{q}_{D,k} = -\boldsymbol{K}_{\boldsymbol{D}}(\boldsymbol{u}_k)\boldsymbol{\bar{u}}.$ 

With the care of using Eq. (A.15) instead of Eq. (A.7), and remembering to set the imposed degrees of freedom to the proper values after the solution of the condensed systems, the arc-length algorithm can be generalized to Dirichlet boundary conditions.

The arc-length algorithm is summarized in Algorithm 1 for case of mixed Neumann and Dirichlet boundary conditions.

# Algorithm 1 Arc-length algorithm for mixed Neumann-Dirichlet boundary conditions.

Given  $s_0 = 0$  and  $\boldsymbol{u}_0$ , do: 1.  $\boldsymbol{R}_k = \boldsymbol{F}^{int}(\boldsymbol{u}_k) - s_k \boldsymbol{q}_N$ ; 2. Solve for  $\delta \boldsymbol{u}_{\boldsymbol{R},k}$ : $\boldsymbol{K}_{\boldsymbol{N}}(\boldsymbol{u}_k) \ \delta \boldsymbol{u}_{\boldsymbol{R},k} = -\boldsymbol{R}_k$ ; 3. Solve for  $\boldsymbol{u}_{\boldsymbol{q},k}$ : $\boldsymbol{K}_{\boldsymbol{N}}(\boldsymbol{u}_k) \ \boldsymbol{u}_{\boldsymbol{q},k} = \boldsymbol{q}_N + \boldsymbol{q}_{D,k}$ ; 4. Solve for  $\delta s_{k+1}$ : $a \ (\delta s_{k+1})^2 + 2b \ \delta s_{k+1} + c = 0$ ; 5.  $\delta \boldsymbol{u}_{k+1} = \delta s_{k+1} \boldsymbol{u}_{\boldsymbol{q},k} + \delta \boldsymbol{u}_{\boldsymbol{R},k}$ ; 6.  $\boldsymbol{u}_k \leftarrow \boldsymbol{u}_k + \delta \boldsymbol{u}_{k+1}$ ;  $s_k \leftarrow s_k + \delta s_{k+1}$ ;  $k \leftarrow k + 1$ ; 7. Evaluate convergence criterion.If not satisfied, go to Step 1.

In Algorithm 1,  $q_N$  is the direction of the applied external force through Neumann boundary conditions. Notice that the absence of  $q_D$  in the right hand side of Step 2 means that the equation is solved for  $\delta u_{R,k}$  with homogeneous Dirichlet boundary conditions, whereas Step 3 clearly solved with  $u_{q,k}$  being set to  $\bar{u}$  on the Dirichlet boundary. As a consequence, and as it is desired, the boundary value of  $\delta u_{k+1}$  in Step 5 is  $\delta s_{k+1} \bar{u}$ .

The iterative algorithm described above can be initialized at the very first load step with  $u_0 = 0$  and  $s_0 = 0$ . With this choice,  $\mathbf{R}_0 = \mathbf{0}$  and Step 2 is trivial ( $\delta u_{\mathbf{R},0} = \mathbf{0}$ ), Step 3 remains unchanged, while in Step 4 the equation simplifies, being b = 0 and  $c = -\Delta l^2$ . As a consequence, at the first nonlinear iteration of the first load step, the arc-length Eq. (A.11) simplifies into:

$$\Delta l = \sqrt{\psi^2 \ \eta^2 + ||\mathbf{u}_{q,0}||^2} \ \delta s_1 = \eta \sqrt{1 + \psi^2} \ \delta s_1. \tag{A.16}$$

Eq. (A.16) is very useful, as it gives a rule of thumb on the selection of the arc-length parameter  $\Delta l$ . In fact, compared to the load factor increment at the first nonlinear iteration of the first load step  $\delta s_1$ ,  $\Delta l$  has a less intuitive physical meaning. As a consequence, instead of choosing a value for  $\Delta l$ , we set an initial load factor  $\delta s_1$  based on which the arc-length parameter  $\Delta l$  can be easily computed with Eq. (A.16).

The arc-length measure  $\Delta l$  can be adaptively modified during the simulation depending on the problem specifications. In the literature, several techniques for arc-length adaptivity have been proposed, (Crisfield, 1981a; Yang and Chen, 2004; Yuanqi and Zuyan, 2004). Here, we adopt the formulation presented in Yang and Chen (2004), *i.e.* 

$$\Delta l = \left(\frac{n_D}{n^{old}}\right)^M \Delta l^{old},\tag{A.17}$$

where  $\Delta l$  and  $\Delta l^{old}$  denote the arc measures of two consecutive load iterations, the exponent *M* ranges between 0.25 and 0.5, whereas  $n_D$  is the desired number of iterations for the nonlinear solver to converge. Analogously,  $n^{old}$  represents the number of iterations needed for convergence in the previous load step.

One nontrivial aspect of Crisfield's approach is the proper choice of a solution to the quadratic scalar Eq. (A.11). The choice is trivial at the beginning of the simulation and we choose the solution  $\delta s$  that leads to an increment of the load. However, the selection process between two consecutive arc-length iterations is not trivial in general, de Souza Neto and Feng (1999); Vasios (2015). We follow here the solution proposed in Vasios (2015) and we choose  $\delta s_{k+1}$  that maximizes the quantity:

$$P = (\Delta \boldsymbol{u}_k + \delta \boldsymbol{u}_{k+1}) \cdot \Delta \boldsymbol{u}^{old} + \psi^2 \eta^2 (\Delta s_k + \delta s_{k+1}) \Delta s^{old},$$
(A.18)

where  $\Delta u^{old}$  and  $\Delta s^{old}$  denote the converged increments from the previous nonlinear iteration. In Eq. A.18, *P* represents the projection, in the sense of a metrics defined by the arc-length function, of the newly computed value of the increments  $\Delta u_{k+1}$  and  $\Delta s_{k+1}$  with respect to the values of these increments at the previous load step.

Finally the stopping criterion used to assess convergence in the iterative procedure is stated as follows:

$$\frac{\sqrt{||\delta \boldsymbol{u}_{k+1}||^2 + \psi^2 \eta^2 \delta s_{k+1}^2}}{\Delta l} < \text{tol.}$$
(A.19)

## Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.jmps.2019.06.020

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