How to accelerate and improve the continuation algorithm called ANM ?

How to move from real to complex continuation ?

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Outline

- Introduction.
- How to improve the convergence of Taylor series ?
- Convergence acceleration MMPE.
- Technique of adaptative steps.
- Numerical results.
- Recent developments : complex continuation using ANM
- Conclusions and perspectives.

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Introduction

- The purpose: solve $\mathbf{R}(\mathbf{u},\lambda)=\mathbf{0}$, with $\mathbf{R}$, $\mathbf{u}, \in \sim^{n}$ and $\lambda \in \sim$

$\mathbf{R}$ is a continuously differentiable and analytic function

when $\dfrac{\partial \mathbf{R}}{\partial u}\left(\mathbf{u}^{J},\lambda^{J}\right)$ is invertible $\Rightarrow$ solution $\mathbf{u}(\lambda)$ in the neighborhood of $\left(\mathbf{u}^{J},\lambda^{J}\right)$

- The **Asymptotic Numerical Method** (**ANM**) is a continuation method that relies on a perturbation technique based on an expansion with **Taylor series** (using a path parameter) of the solution vector and of the load parameter.

  Reference : *B. Cochelin, N. Damil, M. Potier-Ferry, Méthode Asymptotique Numérique, Hermès Lavoisier, 2007*.

- **ANM** has been widely used for non linear elasticity, non linear vibration …

- **Its main interest**: by allowing to adjust the step length the **ANM** brings a close follow up of the curves with bifurcations.

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Introduction

- We are going to present big improvements of the algorithm of **ANM** :

  - Convergence acceleration of the **ANM** continuation with the help of **MMPE** (**M**odified **M**inimal **P**olynomial **E**xtrapolation) technique.
  - Implementation of the step length adaptation.
  - **Newton-Riks corrections** at the end of the **ANM** continuation phase.

- This research has been published in Comptes Rendus Mécanique de l'Académie des Sciences, 348, **issue 5** (2020), p. 361-374.

P. Ventura, M. Potier-Ferry, and H. Zahrouni, "A secure version version of the Asymptotic Numerical Method via convergence acceleration".

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Introduction

- **ANM** is well suited to the study of instabilities problems in mechanics like the wrinkles in film/substrate systems, which requires many **ANM** steps and a huge number of degrees of freedom, but leads to a slowly loss of accuracy when chaining steps.

- Finite element method has been used to simulate wrinkles in film/substrate systems. It is more suited than spectral methods to simulate complex geometries and any boundary conditions.

- A 3D finite element software implementing **ANM** has been used. It is developped using **FreeFem++** with parallel (MPI) computational capababilities.

P. Ventura, M. Potier-Ferry, H. Rezgui-Chaabouni, F. Xu, and, F. Hecht, "Analyse 3D des plissements dans les systèmes film/substrat à l'aide de la MEF et de la MAN", congrès CSMA 2019.

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Convergence improvements of Taylor's series

- Solving non linear problems using **ANM** consists in chaining steps.

- Each step consists in a truncated Taylor series of vectors :

$$a \in {}^{\sim} \rightarrow \mathbf{U}(a, N) = \sum_{n=0}^{N} a^n \mathbf{U}_n$$

- A user parameter δ , related to the difference between $\mathbf{U}(a, N)$ and $\mathbf{U}(a, N-1)$, allows to make the choice between a short or large steps strategy.

- For each δ , a parameter $a_{\max}$ is evaluated which allows to define the validity range of the serial, and so the path of the local branch of the **ANM** step.

- In most of the cases, when chaining several **ANM** steps, a slow deterioration of the accuracy of the ANM continuation is observed.

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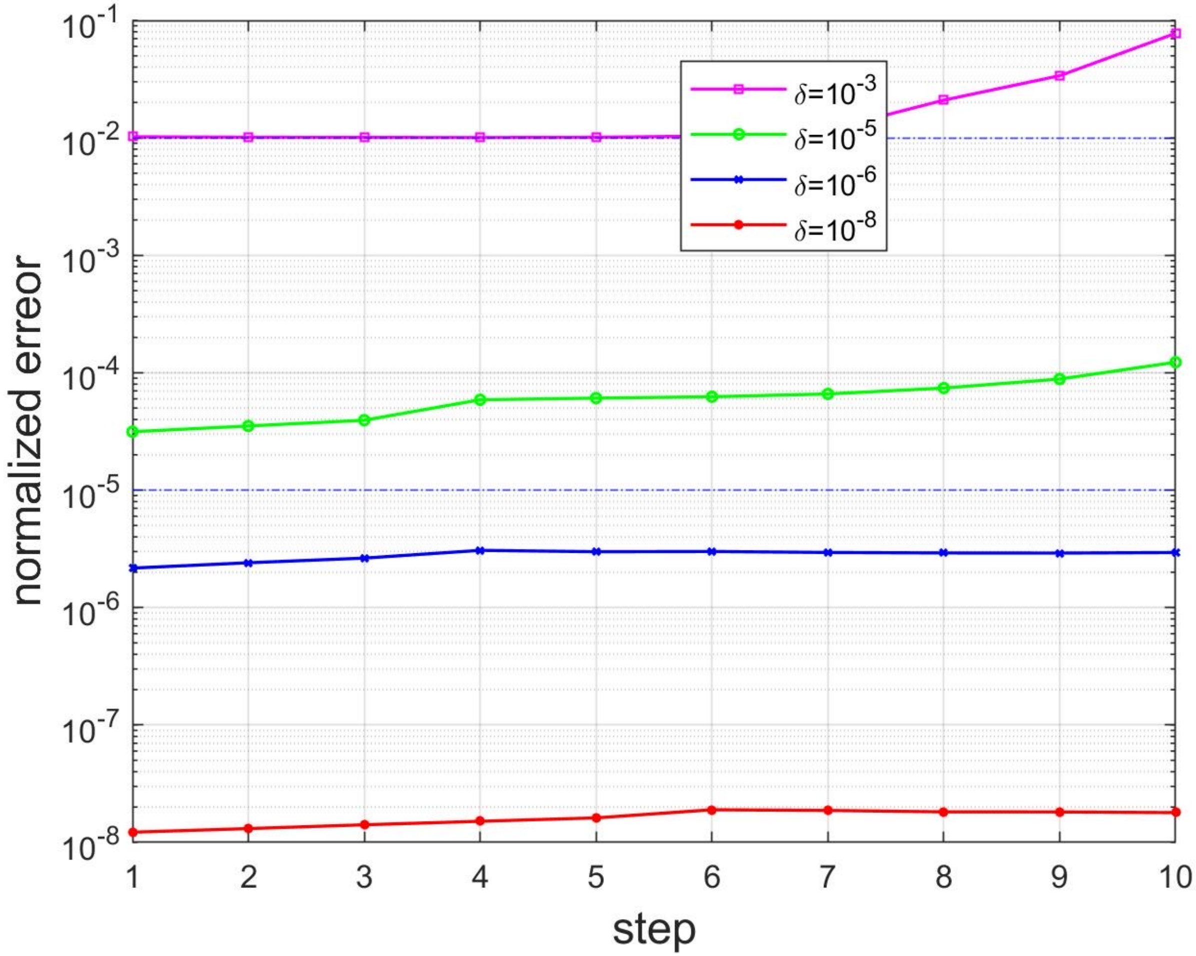
Convergence improvements of Taylor's series



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Convergence improvements of Taylor's series

- The more natural way to control the accuracy of the **ANM** continuation is to introduce **Newton-Riks corrections** phases at the end of each **ANM** step, when needed. But, this technique increases a lot CPU time.

- **Padé approximant** method (interpolation with rational fractions), has also been proposed as a continuation method in the case of non linear shell analysis, contact mechanics, hyperelastic structures, bifurcation in fluid mechanics.

- But, we need to be careful with **Padé approximant** method because of the presence of spurious pole of rational fractions.

- Many convergence acceleration techniques exist, the most attractive belongs to the class of vector extrapolation called **MMPE : Modified Minimal Polynomial Extrapolation**.

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Convergence improvements of Taylor's series

- The end step parameter $a_{\max}$ of **ANM** for each Taylor series $\mathbf{U}(a, N)$ is obtained using a user parameter δ :

$$a_{\max} = \left(\delta \frac{\|\mathbf{U}_1\|}{\|\mathbf{U}_N\|} \right)^{1/(N-1)}$$

$$\begin{cases} 10^{-6} \leq \delta \leq 10^{-3} \rightarrow \text{Large step strategy} \\ 10^{-10} \leq \delta \leq 10^{-6} \rightarrow \text{Small step strategy} \end{cases}$$

- Another end step parameter based on the residual has been proposed, it could be implemented later.

- In order to minimize the number of Newton's correction at the end of **ANM** step, we implement a convergence acceleration technique of the vectors sequence $\mathbf{V}_n = \mathbf{U}(a, n)$ when the parameter a is close to $a_{\max}$.

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Convergence acceleration MMPE

- The convergence acceleration, belonging to the class of vector extrapolation **MMPE** (**M**odified **M**inimal **P**olynomial **E**xtrapolation) has been described in the article :

K. Jbilou, H. Sadok, "Vector extrapolation methods, applications and numerical comparison", J. Comput. Appl. Math. ***122*** *(2000), p. 149-165.*

- Let us consider the sequence of vectors $\mathbf{S}_N = \sum_{n=0}^{N} \mathbf{V}_n$ with $\mathbf{V}_0 = \mathbf{S}_0$ and $\mathbf{V}_n = \mathbf{S}_n - \mathbf{S}_{n-1}$. The sequence of vectors $\mathbf{V}_n$ appears naturally in the Taylor series expansion of **ANM** .

- **MMPE** introduces a sequence of modified vectors : $\mathbf{T}_N = \mathbf{S}_0 + \sum_{n=0}^{N} c_n \mathbf{V}_n$

- Then we use a shift of index : $\tilde{\mathbf{T}}_N = \mathbf{S}_1 + \sum_{n=1}^{N} c_n \mathbf{V}_{n+1}$

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Convergence acceleration MMPE

- Let us introduce a family of independent vectors $\{\mathbf{Y}_1, \mathbf{Y}_2, \cdots, \mathbf{Y}_N\}$ with $\mathbf{Y}_n = \mathbf{V}_n^*$ where $\{\mathbf{V}_1^*, \mathbf{V}_2^*, \cdots, \mathbf{V}_N^*\}$ is obtained using **Gramm Schmitt orthogonalisation** of the family of vectors $\{\mathbf{V}_1, \mathbf{V}_2, \cdots, \mathbf{V}_N\}$

- The number of vectors is often in the range 6-15 for avoiding the loss of accuracy.

- The coefficients $\{\mathbf{c}\}$ are obtained by asking that the residual $\left(\tilde{\mathbf{T}}_N - \mathbf{T}_N\right)$ is orthogonal to the vectorial space spanned by $\{\mathbf{Y}_1, \mathbf{Y}_2, \cdots, \mathbf{Y}_N\}$.

- We solve the linear system: $$[\mathbf{M}]\{\mathbf{c}\} = \{\mathbf{b}\}$$

  with , $\{\mathbf{c}\} = {}^t\{c_1, c_2, \cdots, c_N\}$, $M_{ij} = \left(\mathbf{V}_{j+1} - \mathbf{V}_j\right) \cdot \mathbf{Y}_i$, and, $b_i = -\mathbf{V}_1 \cdot \mathbf{Y}_i$

- **MMPE** consists in solving a small linear system which has a small impact on the increase of CPU time.

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Adaptative step technique

- In the **ANM**, the step length is given by the parameter $a_{\max}$ and the formula used to compute it from Taylor series is the same for all the steps.

- In practice, a more adaptative algorithm will be more interesting.

- In fact, the loading curve shows alternation of slow variation parts for which it would be possible to increase the step and sharp variation parts (close to bifurcations) for which it would be possible to shorten the step.

Improved Continuation Algorithm

(1) Compute the Taylor series $\mathbf{U}(a,N)$.

(2) Compute the validity range $a_{\max}$ of this series and compute the residual.

(3) Apply **MMPE** to a family of points $\mathbf{U}(a,N)$, $a = ra_{\max}$, $r \in \{0.7, 0.8, 0.9, 1., 1.1, 1.2, 1.3\}$

Therefore, **ANM** gives 7 points $\mathbf{U}(ra_{\max}, N)$ and 7 additional points are obtained when applying **MMPE** acceleration technique.

(The accuracy parameters ε_1 and ε_2 are used for example $\varepsilon_1 = 10^{-5}$ and $\varepsilon_2 = 10^{-6}$)

(4) Among the 14 test solutions, we keep the one for which the residual error is smaller than ε_2 and the step is maximum. If it is not possible, but if the smallest residual is between ε_2 and ε_1, this solution is kept. In both cases, pass to the next step.

(5) If none of the 14 test solutions get a residual error smaller than ε_1, it is necessary to make **Newton-Riks corrections** until les residual error is smaller than ε_2.

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Numerical results

- High computational capabilities are often needed for the numerical simulation of **film-substrate systems**.

X. Chen, J. W. Hutchinson, "Herringbone buckling patterns of compressed thin films on compliant substrate", J. Appl. Mech. ***71*** *(2004), p. 597-603.*

- Film and substrate are meshed with volumic finite éléments (tetraedral) , Lagrange P2.

- Linear approximation for the substrate and geometrical non linearities are assumed for the film. We also assume Saint Venant Kirchhoff elasticity.

- The convergence acceleration algorithm has been implemented if the **FreeFem++ environment**:

- The 3D finite element model leads to a huge number of degrees of freedom, which allow to show the interest for the new convergence acceleration algorithm for **ANM**.

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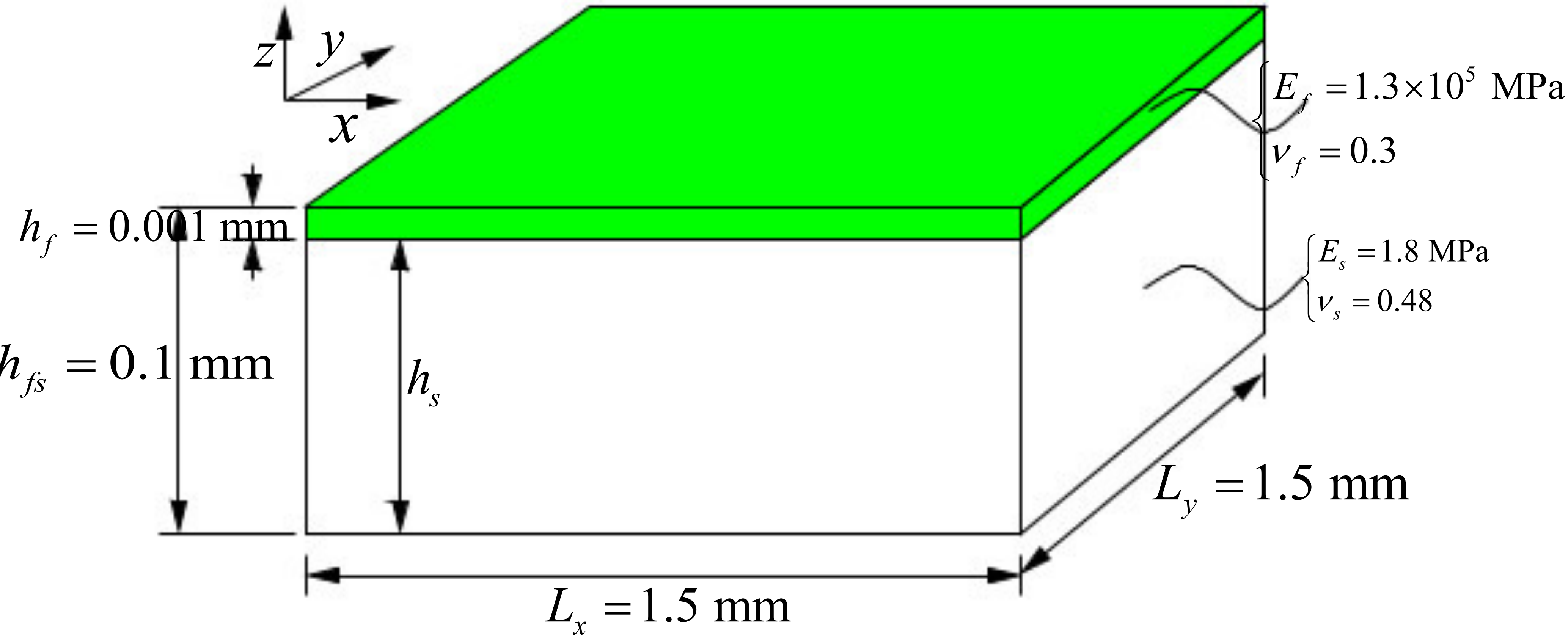
Numerical results



very stiff $E_f / E_s = 72222$

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Numerical results

- Same assumptions, boundary conditions, and, symmetry planes than in the article :

F. Xu, M. Potier-Ferry, S. Belouettar, Y. Cong, "3D finite element modeling for instabilities in thin films and soft substrates", Int. J. Solids Struc. 51 (2014), p. 3619-3632.

- Only a quarter of the structure is meshed, the vertical displacement is blocked on the bottom, a lateral uniaxial force is applied on the lateral face of the film where the y and z displacements are blocked.

- The mesh consists in 100 elements for the lenght, and the width, 5 elements for the heigth, and 1 element for the film thickness.

- The software has been run in parallel (MPI) on 4 processors, 55 Go of memory is needed, the CPU time for one **ANM** step is approximatively 55 minutes.

- CPU time of **Newton-Riks** iterations is important because in the **ANM** algorithm most of CPU time is due to tangent matrix factorization.

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Numerical results

- A reference computation is done for the improved algorithm, $\delta = 10^{-6}$ with 200 ANM steps.

- First, computations with **only ANM continuation**, without **Newton-Riks** corrections, for 100 ANM steps with

$$\delta \in \left\{10^{-3}, 10^{-5}, 10^{-6}, 10^{-8}\right\}$$

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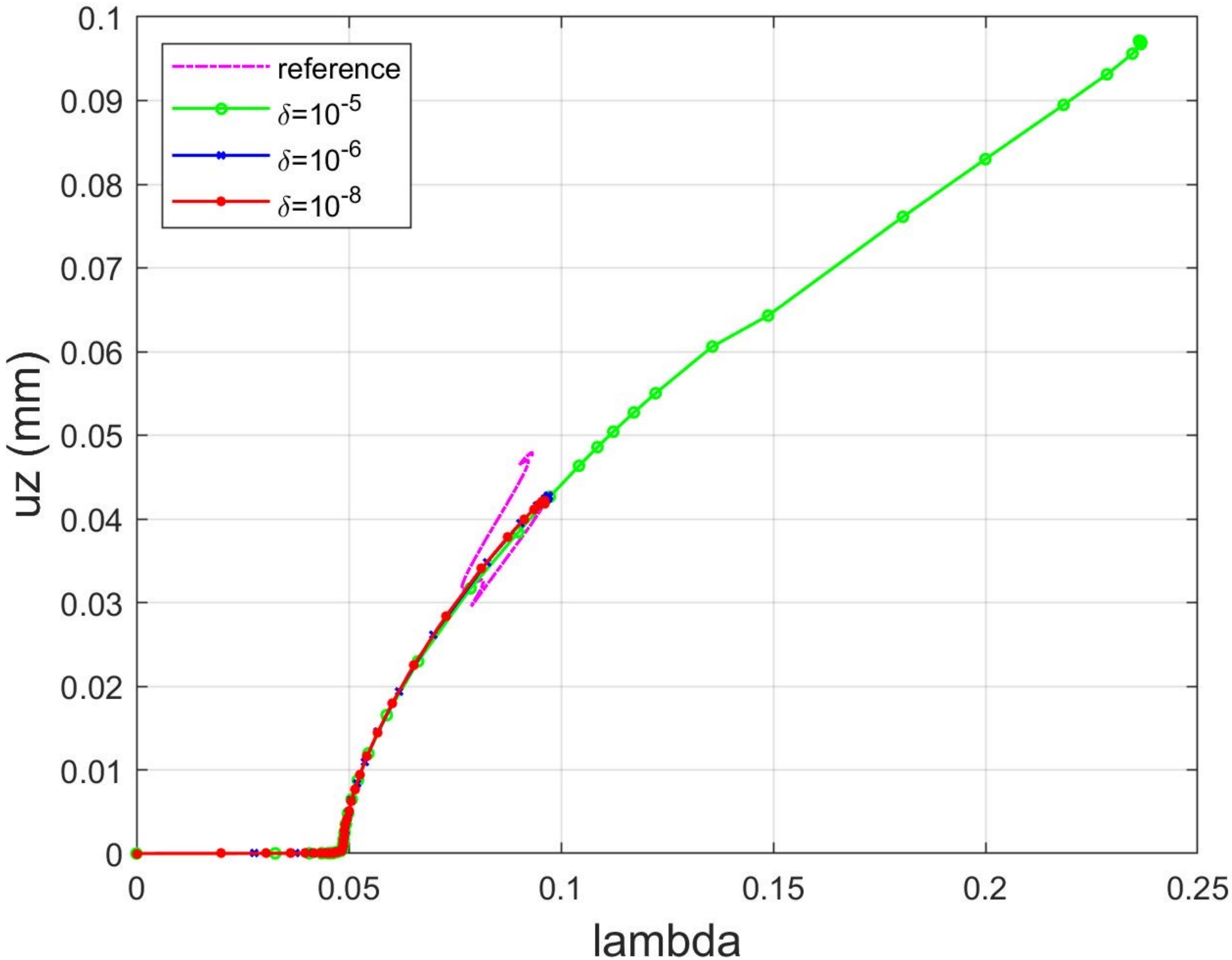

Bifurcation diagram : vertical displacement of the middle of the film (top surface), using only ANM continuation. Comparison with the reference computation

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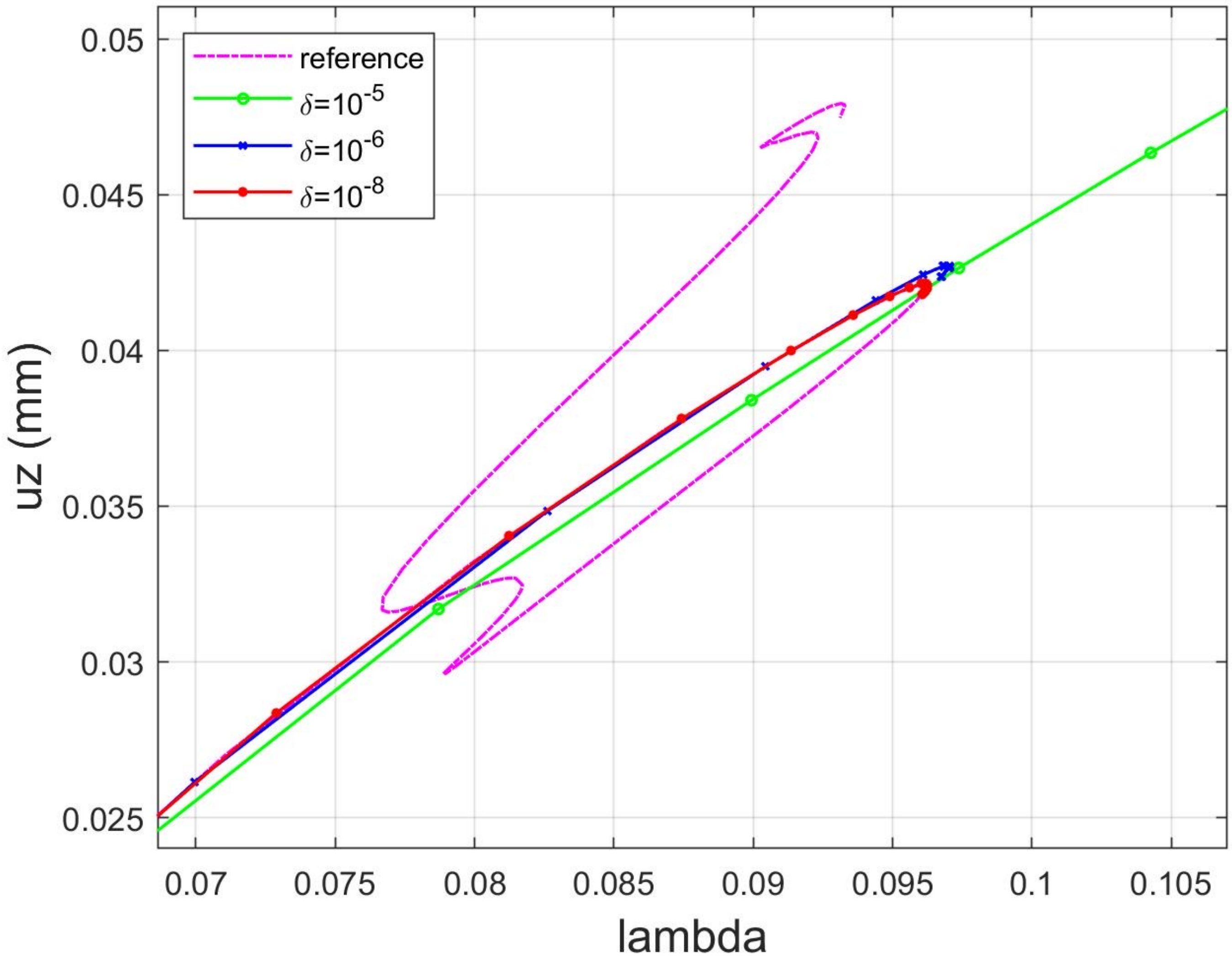

Bifurcation diagram (zoom): vertical displacement of the middle of the film (top surface), using only ANM continuation. Comparison with the reference computation

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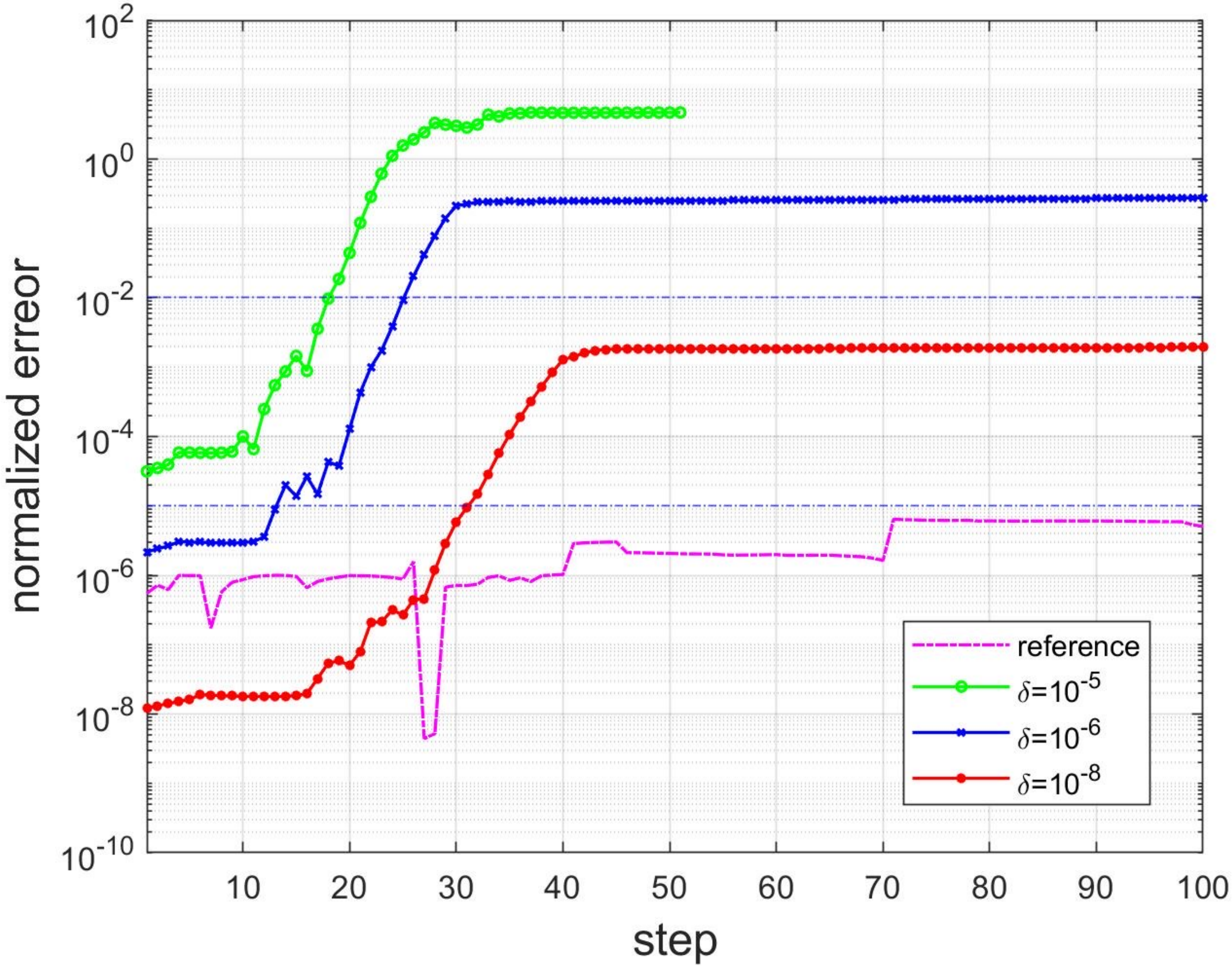

Normalized residual error using only ANM, and comparison with the reference computation. Newton-Riks iterations are needed to reach a good accuracy after the ANM step 20 !

Numerical results

- **Strategy 1** : **Newton-Riks corrections** when the normalized residual error is greater than $\varepsilon_1 = 10^{-5}$
  The number of Newton-Riks corrections per step is below 1 or 2.

- **Strategy 2 : optimized algorithm** : add convergence acceleration phase MMPE with $\varepsilon_2 = 10^{-6}$

δ	10^{-5}	10^{-6}	10^{-8}
Pure Newton	115	87	53
Full algorithm	5	2	0

Total number of Newton-Riks corrections

- For the optimized algorithm, we see a great efficiency of the convergence acceleration (no need of Newton's correction) and because of the step length adaptation the step length is often increased ($r > 1$).

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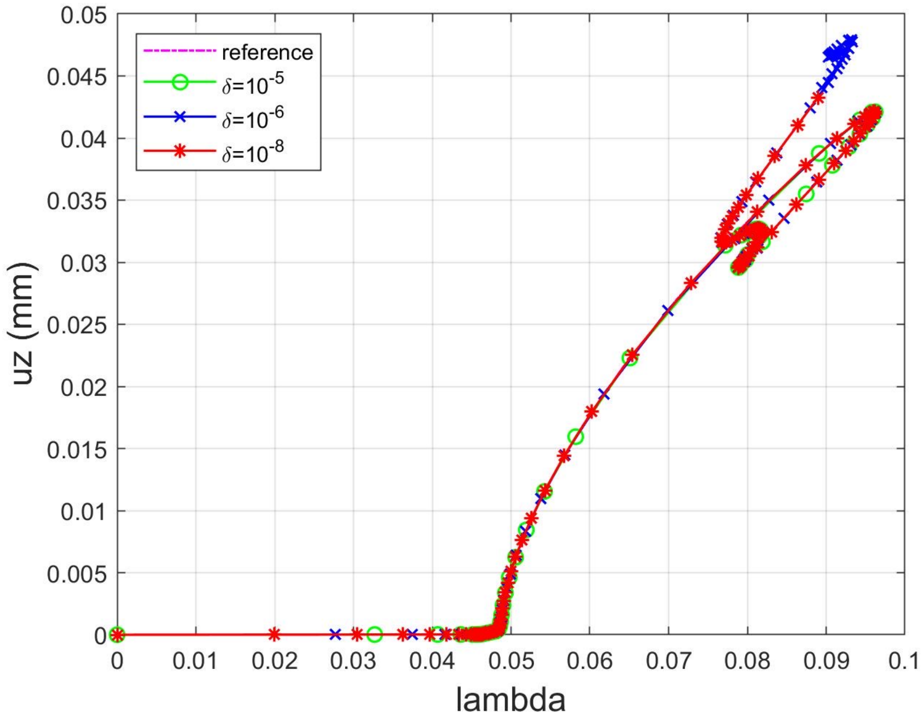
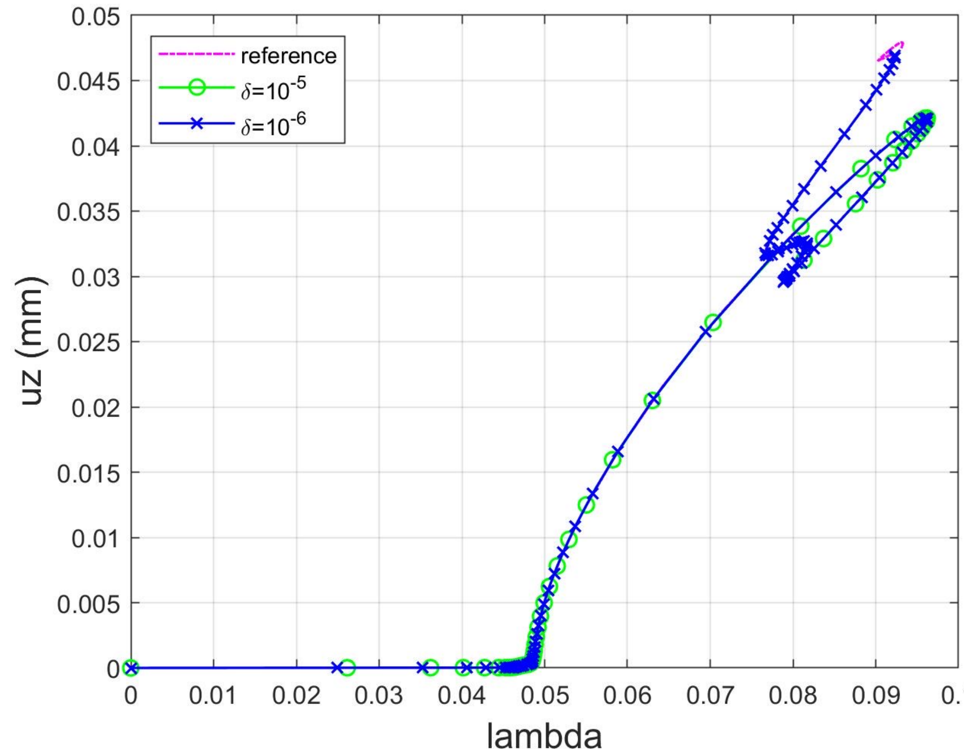


Without step adaptation



With step adaptation

100 ANM steps with
Newton Corrections

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Numerical results

- In order to show the interest of convergence acceleration technique, a typical example at step 34 is detailed: ($\delta = 10^{-6}$)

r	0.7	0.8	0.9	1	1.1	1.2	1.3
Before MMPE	9.01E-6	7.40E-5	4.90E-4	2.66E-3	1.22E-2	4.92E-2	1.77E-1
After MMPE	9.35E-7	9.84E-7	2.36E-6	1.38E-5	7.57E-5	3.65E-4	1.58E-3

- Great efficiency of the MMPE acceleration technique.

- The implementation of the convergence acceleration MMPE, of the step adaptation and of Newton-Riks corrections allows to create a reliable and efficient procedure based on ANM.

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Numerical results

- Caracterization of the wrinkles in film/substrate systems.
- The same reference computation as previously 200 ANM steps, $\delta = 10^{-6}$
- The animation illustrates the evolution of the wrinkles as a function of the ANM steps.

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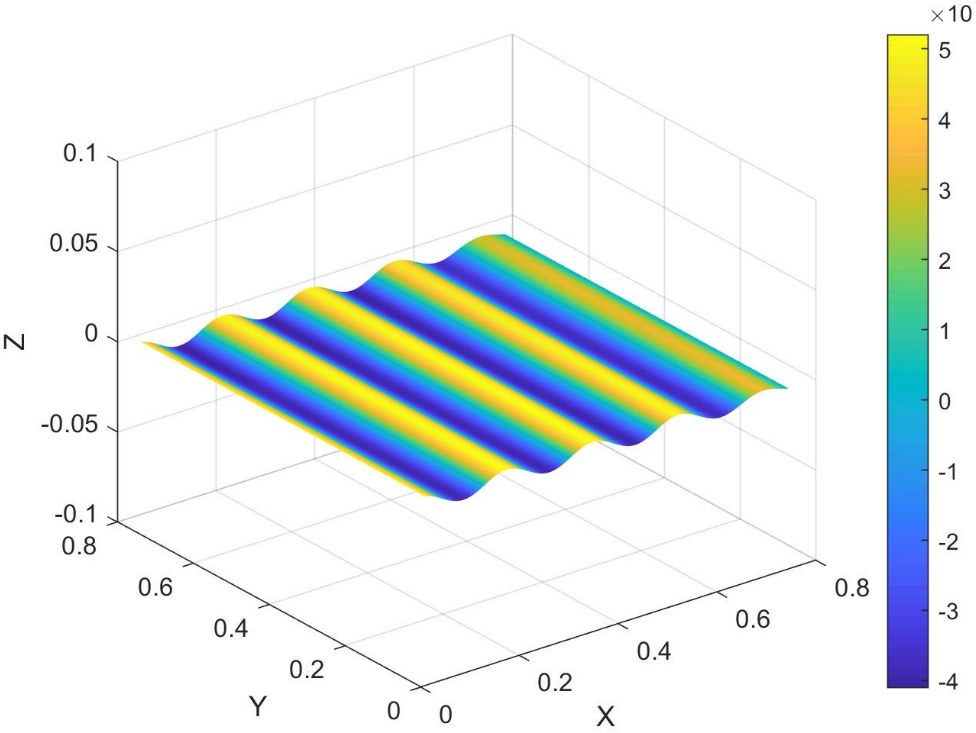
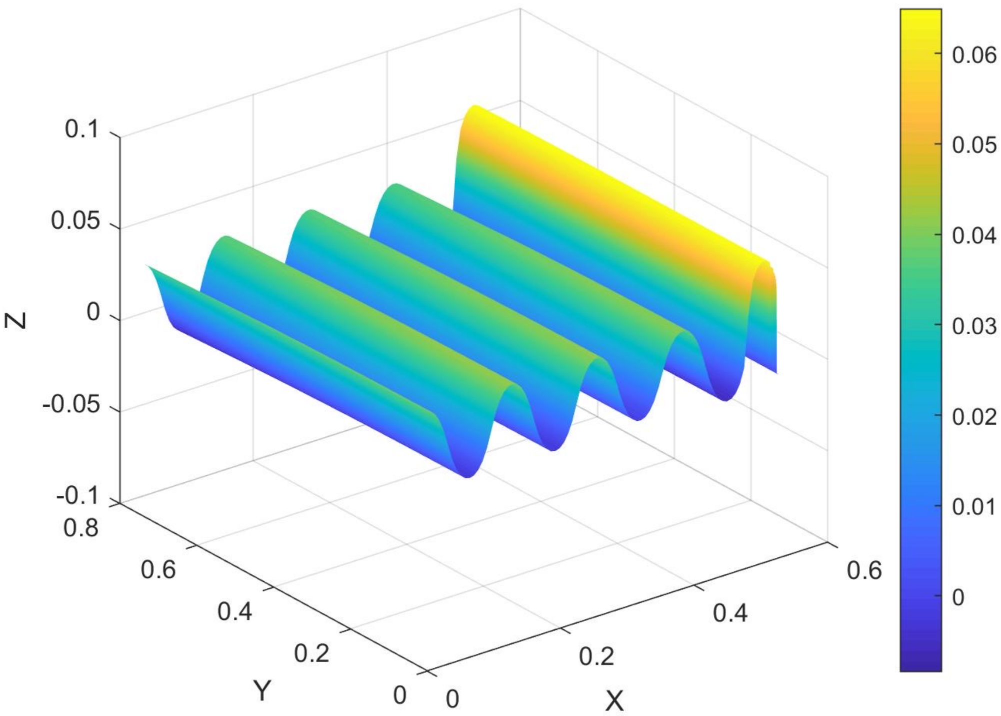


Just after bifurcation : step 20



Just before the first turning point: step 34

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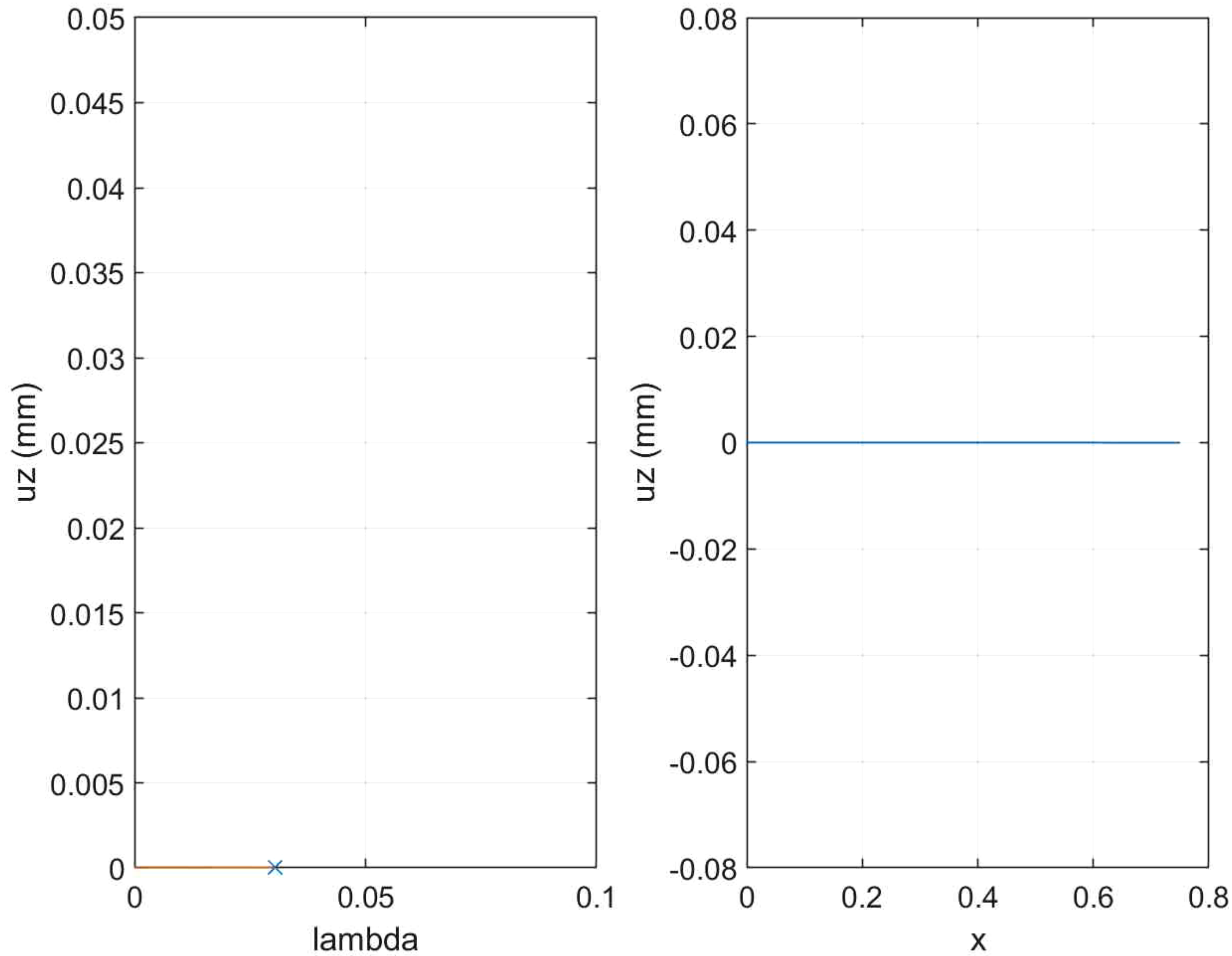

Animation : bifurcation diagram and deformation of the top surface

Complex Continuation using ANM

- First researches regarding complex continuation have been done by Henderson and Keller : ″Complex Bifurcation from real paths″ SIAM Journal on Applied Mathematics″, 50(2), 460-482.

- The basic idea is simply that real solution paths of real analytic problems frequently have complex paths bifurcating from them. Henderson called this phenomena : complex bifurcation.

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Complex Continuation using ANM

- First results obtained using **ANM complex continuation** for the problem of the thermo-mechanical skrinkage of the core of a film/substrate ball. Geometrical non linearities are assumed for the film, while for the core linear elasticity is assumed.

- In the core domain, the thermo-mechanical shrinkage is taken into account using the relationship:

$$\mathbf{S} = \mathbf{D} : \left(\gamma\left(\mathbf{u}\right) - \lambda \mathbf{I} \right)$$

- The **real** variational formulation is modified by introducing **complex** displacement fields, which results in doubling the number of degrees of freedom at each node:

$$\mathbf{u} = \mathbf{u}_r + i\mathbf{u}_i$$

- Let us notice that scalar products are transformed to hermitian product.

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Complex Continuation using ANM

- In a generic way, the real variational problem can be modelled:

$$L(\mathbf{U})+Q(\mathbf{U},\mathbf{U})-\lambda\mathbf{F}=0 \qquad \mathbf{U}=\begin{pmatrix}\mathbf{u}\\ \mathbf{S}\end{pmatrix}$$

where, L is a linear form, Q is a quadratic form .

with the associated weak forms: $\langle L(\mathbf{U}),\delta\mathbf{U}\rangle$, $\langle Q(\mathbf{U},\mathbf{U}),\delta\mathbf{U}\rangle$, and, $\langle \mathbf{F},\delta\mathbf{U}\rangle$

- Derivation of the complex variational form is obtained:

$$\mathbf{U}=\mathbf{U}_r+i\mathbf{U}_i \quad \delta\mathbf{U}=\delta\mathbf{U}_r+i\delta\mathbf{U}_i \quad \langle .,.\rangle$$ Hermitian product

- Real and imaginary part of the complex variational formulation are used to derive the final variational formulation.

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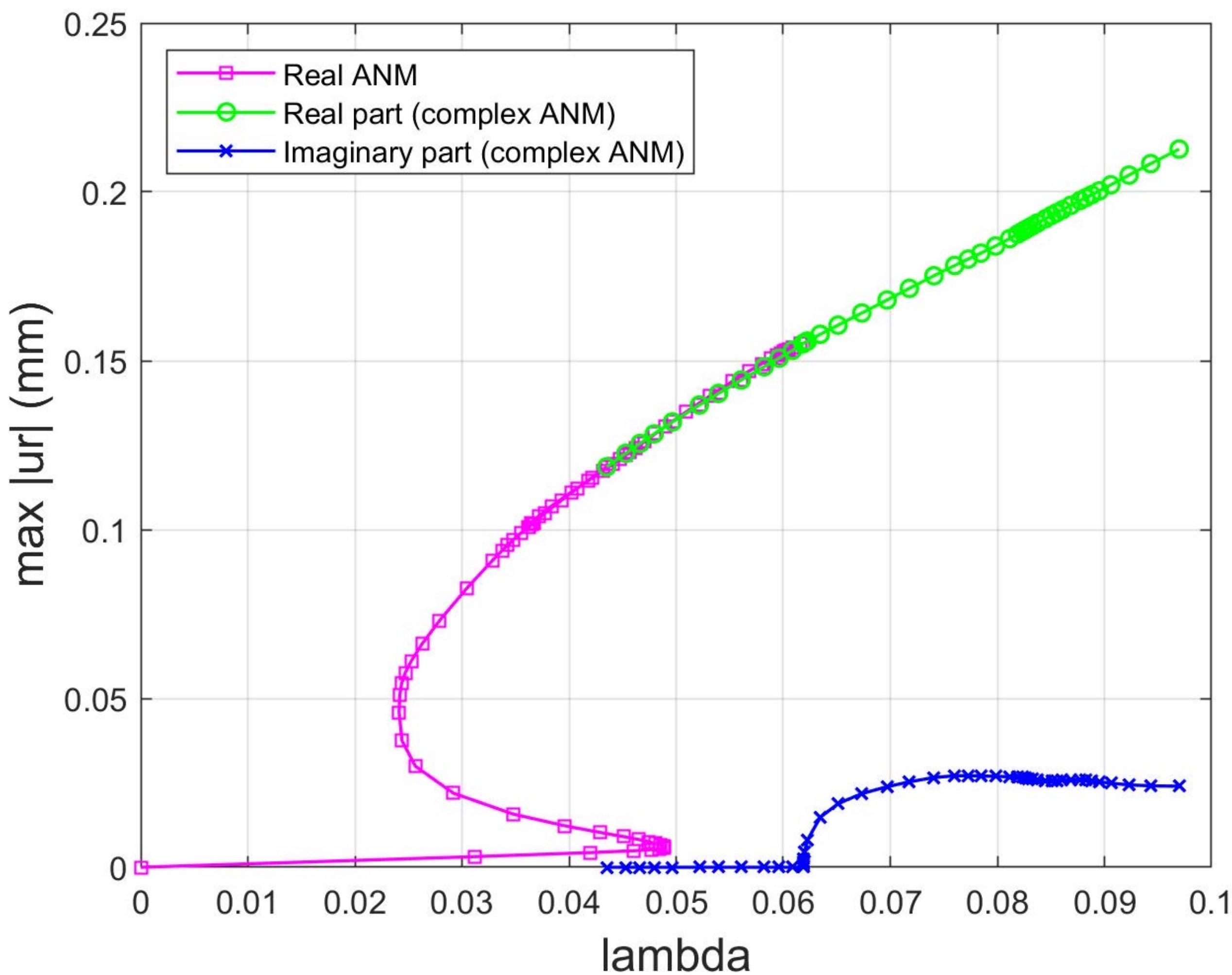
Complex Continuation using ANM



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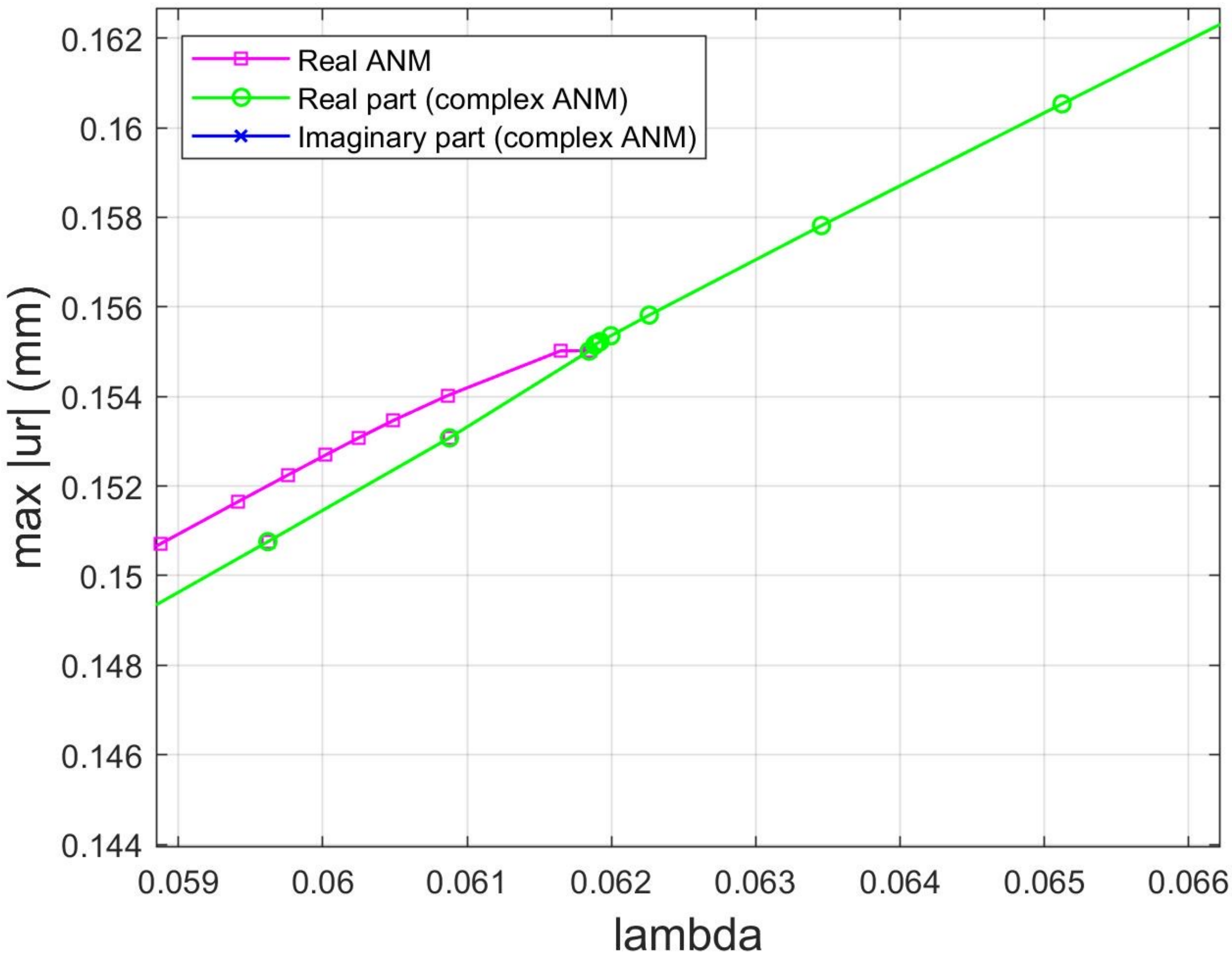
Complex Continuation using ANM



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Conclusions

- We have discussed new techniques around **ANM**, and it appeared that Newton-Riks corrections are necessary in order to avoid the loss of accuracy due to the chaining of the **ANM** steps.

- This simple prediction correction method has been completed using two inexpensive techniques: the convergence acceleration **MMPE** and a step length adaptation based on the residual.

- Great efficiency of the improved algorithm, which eliminates almost all Newton Riks correction, and also to optimize the step length.

- Interesting results have been obtained regarding the study of the wrinkles in the film/substrate systems: The loading curve shows several hysteris loops in the range $u_z/h_f \simeq 40$ related to the growth of a single wrinkle near the boundary of the film and to the unfinished disappearance of one wrinkle during the loading process.

- Based on the Henderson's research that states that real solution paths of real analytic problems frequently have complex paths bifurcating from them, we have beginning to develop a complex continuation algorithm using ANM.

- First results for complex continuation have been obtained for the thermo-mechanical shrinkage of a ball film/substrate.

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Perspective

- Create a documented module in website https://freefem.org.

- With the help of Pierre Jolivet develop a multi grid parallel version (PETSc) able to take into account very large problems (film/substrate systems with many wrinkles).

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