Nonlinear analysis of wrinkles in film-substrate systems by Finite Element Method and Asymptotic Numerical Method using FreeFem++

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Outline

- Introduction.
- Asymptotic Numerical Method for elastic nonlinear problems.
- How to add thermo-elasticity in the ANM ?
- Implementation of the ANM for solid mechanics in FreeFem++.
- Numerical results.
- Conclusions and perspectives.

Introduction

- Wrinkling phenomena of thin membranes or film-substrate systems are very common in the recent literature.

- Numerical modeling of these instabilities may be highly complicated due to the existence of many equilibrium solutions.

- It is not easy to apply a continuation algorithm that may fails.

- Asymptotic Numerical Method (ANM) is a continuation method based on Taylor series. It is associated with classical discretization techniques, generally the Finite Element Method (FEM).

- The coupling between perturbation technique and FEM was first proposed by Thompson and Walker [1]. A continuation method together with an efficient procedure to build the Taylor series and convergence acceleration by Padé approximants were introduced By Cochelin, Damil and Potier-Ferry [2].

[1] J. M. T. Thompson, A. C. Walker, The non-linear perturbation analysis of discrete structural systems, International Journal of Solids and Structures, 1968, vol. 4, pp.757-768.

[2] B. Cochelin, N. Damil, M. Potier-Ferry, The asymptotic numerical method: an efficient technique for nonlinear structural mechanics, Revue Européenne des Eléments Finis, vol. 3, pp. 281-297, 1994.

Introduction

- ANM is rather different from classical incremental-iterative methods because full solution paths are computed and not only pointwise solutions and because an estimate of the radius of convergence yields the step length a posteriori, which ensures optimal control of step sizes.

- Many home-made implementations of ANM have been done: MANLAB [3] is widely used in the field of nonlinear vibration. Lejeune et al. developed a full object-oriented implementation within C++ [4].

[3] C. R. Arquier, B. Cochelin, Manlab, URL http://manlab.lma.cnrs.fr/

[4] A. Lejeune, F. Béchet, H. Boudaoud, N. Mathieu, M. Potier-Ferry, Object-oriented design to automate a high order nonlinear solver based an asymptotic numerical method, Advances in Engineering Software 48 (2012) 70-88.

- The C++ implementation makes it difficult to implement new features and it would be preferable to work in a user-friendly framework. Here, the implementation of ANM in the FreeFem++ code is discussed.
- FreeFem++ uses a high level language that allows to derive very easily variational formulation and to implement the ANM algorithm.

- Computational results will be shown in the case of both a planar film/substrate system under uni-axial loading, and, of a spherical film/substrate subjected to a thermo-mechanical shrinkage of its compliant core.

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ANM for elastic nonlinear problems

- Let us presents the basics of ANM in the case of geometrically nonlinear elasticity.
- We consider an elastic domain that obeys Saint-Venant Kirchhoff law: linear relation between the second Piola-Kirchhoff stress tensor S and the Green-Lagrange strain tensor $\gamma(u)$ defined by:

$$\gamma(u) = \underbrace{\frac{1}{2}\left(\nabla u + \nabla^T u\right)}_{\gamma_l(u)} + \underbrace{\frac{1}{2}\left(\nabla^T u \cdot \nabla u\right)}_{\gamma_{nl}(u)} \qquad (1)$$

And, its variation: $\delta\gamma(u) = \gamma_l(\delta u) + 2\gamma_{nl}(u, \delta u)$ (2)

- The formulation of the problem, including boundary condtitions, is classical and it associates the elastic constitutive law and the virtual work equations:

Elastic stiffness tensor

$$\begin{cases} S = D : \gamma(u) \\ \int_\Omega S : \delta\gamma(u)\, d\Omega - \lambda \int_{\Gamma_D} t \cdot \delta u\, d\Gamma = 0 \end{cases} \qquad (3)$$

Given force on Γ_D

Scalar loading parameter

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ANM for elastic nonlinear problems

- ANM relies on Taylor series according a well-known path parameter a:

$$\begin{cases} \mathrm{u}(a) = \mathrm{u}_0 + a\mathrm{u}_1 + a^2\mathrm{u}_2 + \cdots \\ \mathrm{S}(a) = \mathrm{S}_0 + a\mathrm{S}_1 + a^2\mathrm{S}_2 + \cdots \\ \lambda(a) = \lambda_0 + a\lambda_1 + a^2\lambda_2 + \cdots \end{cases} \qquad (4)$$

- The most popular choice is a linearized arclength parameter that permits to bypass all the extrema of the response curve:

$$a = \frac{1}{\bar{\mathrm{u}}^2}\langle \mathrm{u} - \mathrm{u}_0, \mathrm{u}_1 \rangle + \alpha(\lambda - \lambda_0)\lambda_1 \qquad (5)$$

Normalized displacement vector

Normalized loading parameter

- When Taylor series (4) are substituted in (3) and (5), we obtain a linear system at each order p in a. The equations involving only linear or quadratic terms with respect to the unknown field (u, S) the system can be deduced from the usual Leibnitz rule to compute high order derivatives or equivalently the Taylor coefficients of a product : $(ab)_p = \sum_{r=0}^{p} a_r b_{p-r}$

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ANM for elastic nonlinear problems

- At the order 1 in a, it results: $k(\mathrm{u}_1, \delta\mathrm{u}) = \lambda_1 P_e(\delta\mathrm{u})$
  where the bilinear form $k(.,.)$ is the classical stiffness tangent operator given by:

$$k(\mathrm{u}, \delta\mathrm{u}) = \int_\Omega \Big(\delta\gamma(\mathrm{u}_0) : \mathrm{D} : \big(\gamma_1(\mathrm{u}) + 2\gamma_{\mathrm{nl}}(\mathrm{u}_0, \mathrm{u})\big) + \mathrm{S}_0 : 2\gamma_{\mathrm{nl}}(\mathrm{u}, \delta\mathrm{u})\Big) d\Omega$$ and, $$P_e(\delta\mathrm{u}) = \int_{\Gamma_D} \mathrm{t} \cdot \delta\mathrm{u}\, d\Gamma$$

The definition (5) of the path parameter gives an additional equation: $\frac{1}{\bar{\mathrm{u}}^2}\langle \mathrm{u}_1, \mathrm{u}_1 \rangle + \alpha\lambda_1\lambda_1 = 1$

- For $p \geq 1$ $\quad \mathrm{S}_p = \mathrm{D} : \left[\big(\gamma_1(\mathrm{u}_p) + 2\gamma_{\mathrm{nl}}(\mathrm{u}_0, \mathrm{u}_p)\big) + \sum_{r=1}^{p-1} \gamma_{\mathrm{nl}}(\mathrm{u}_r, \mathrm{u}_{p-r}) \right]$
  and we also get at order $p \geq 2$ a variational formulation involving the same bilinear form:

$$k(\mathrm{u}_p, \delta\mathrm{u}) = \lambda_p P_e(\delta\mathrm{u}) + \langle \mathrm{F}_p^{\mathrm{nl}}, \delta u \rangle$$

where the last term is a linear form taken into account the truncation error due to Taylor series (called non linear part of the right hand side).

$$\langle \mathrm{F}_p^{\mathrm{nl}}, \delta u \rangle = -2\sum_{r=1}^{p-1} \int_\Omega S_r : \gamma_{\mathrm{nl}}(\mathrm{u}_{p-r}, \delta\mathrm{u})\, d\Omega - \sum_{r=1}^{p-1} \int_\Omega \gamma_{\mathrm{nl}}(\mathrm{u}_{p-r}, \delta\mathrm{u}) : D : \delta\gamma(\mathrm{u}_0)\, d\Omega$$

Last the arclength condition (5) yields the load parameter λ_p as a function of the displacement u_p:

$$\frac{1}{\bar{\mathrm{u}}^2}\langle \mathrm{u}_p, \mathrm{u}_1 \rangle + \alpha\lambda_p\lambda_1 = 1$$

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ANM for elastic nonlinear problems

- Usually the Taylor expansion order N is chosen between 15 and 50 to take advantage of the exponential convergence of power series. By estimating the convergence radius of the series, it is possible to compute the maximum value $a_{\max}$ of the path for each branch:

$$a_{\max} = \left(\delta \frac{\|\mathrm{u}_1\|}{\|\mathrm{u}_N\|} \right)^{\frac{1}{N-1}}, \text{ with } 10^{-10} \leq \delta \leq 10^{-3}$$

- In this way, the Taylor expansion (4) gives a part of the solution in the interval $[0, a_{\max}]$. The continuation procedure may be very simple by chaining several series, the end point of this path being the starting point of the next step.

- It is also possible to improve the accuracy of the end point by using a corrective step via Newton method or by applying a convergence acceleration technique.

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How to add thermo-elasticity in the ANM

- It is easy to take into account an isotropic thermal expansion (or shrinkage) of an elastic domain with the ANM.
- The thermo-mechanical effects results in an additional contribution $\lambda \mathrm{I}$ to the Green-Lagrange strain tensor.
- Incorporating the thermal effects, the virtual work equation results in:

$$\begin{cases} \mathrm{S} = \mathrm{D} : \left(\gamma_1(\mathrm{u}) + \gamma_{\mathrm{nl}}(\mathrm{u},\mathrm{u}) - \lambda \mathrm{I} \right) \\ \int_\Omega \mathrm{S} : \delta\gamma(\mathrm{u})\, d\Omega = 0 \end{cases}$$

$\lambda \geq 0$, means a thermo-elastic shrinkage

- at the order 1 in a, $k(\mathrm{u}_1, \delta \mathrm{u}) = \lambda_1 P_{\mathrm{th}}(\delta \mathrm{u})$, $P_{\mathrm{th}}(\delta \mathrm{u}) = \int_\Omega \mathrm{I} : \mathrm{D} : \left(\gamma_1(\delta \mathrm{u}) + \gamma_{\mathrm{nl}}(\mathrm{u}_0, \delta \mathrm{u}) \right) d\Gamma$
- For $p \geq 1$ $\quad \mathrm{S}_p = \mathrm{D} : \left[\left(\gamma_1(\mathrm{u}_p) + 2\gamma_{\mathrm{nl}}(\mathrm{u}_0, \mathrm{u}_p) \right) + \sum_{r=1}^{p-1} \gamma_{\mathrm{nl}}(\mathrm{u}_r, \mathrm{u}_{p-r}) - \lambda_p \mathrm{I} \right]$
- At the order $p \geq 2$: $\quad k(\mathrm{u}_p, \delta \mathrm{u}) = \lambda_p P_{\mathrm{th}}(\delta \mathrm{u}) + \langle \mathrm{F}_p^{\mathrm{nl}}, \delta u \rangle$

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Implementation of the ANM for solid mechanics in FreeFem++

- The **ANM** algorithm

Initialize u_0 and λ_0
for step=1 until Nstep
  Assemble $\left[\mathrm{K}_t\left(\mathrm{u}_0,\mathrm{S}_0\right)\right]$ and $\{\mathrm{F}\}$
  Solve $\{\hat{\mathrm{u}}\} = \left[\mathrm{K}_t\left(\mathrm{u}_0,\mathrm{S}_0\right)\right]^{-1}\{\mathrm{F}\}$
  Compute $\lambda_1 = 1\Big/\sqrt{1+\{\hat{\mathrm{u}}\}^T\{\hat{\mathrm{u}}\}}$
  Compute $\{\mathrm{u}_1\} = \lambda_1\{\hat{\mathrm{u}}\}$
  Compute (for each Gauss point $\{\mathrm{S}_1\},\{\mathrm{S}_2^{nl}\}$
  Compute $\{\mathrm{F}_2^{nl}\}$
  for p=2 until N
    Compute $\{\mathrm{u}_p^{nl}\} = \left[\mathrm{K}_t\left(\mathrm{u}_0,\mathrm{S}_0\right)\right]^{-1}\{\mathrm{F}_p^{nl}\}$
    Compute $\lambda_p = -\lambda_1\{\mathrm{u}_p^{nl}\}^T\{\mathrm{u}_1\}$
    Compute $\{\mathrm{u}_p\} = \lambda_p\{\hat{\mathrm{u}}\} + \{\mathrm{u}_p^{nl}\}$
    Compute (for each Gauss point) $\{\mathrm{S}_p\},\{\mathrm{S}_{p+1}^{nl}\}$
    Compute $\{\mathrm{F}_{p+1}^{nl}\}$
  end for
  Compute $a_{\max}$
  Compute $\lambda(a)$ and $\mathrm{u}(a)$ with $a \in [0, a_{\max}]$
  Compute the normalized residual error
  Actualize u_0 and λ_0
end for

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Implementation of the ANM for solid mechanics in FreeFem++

- Macro for differential operators:

```
macro GammaL(u,v,w) [dx(u),dy(v),dz(w),(dy(u)+dx(v)),(dz(u)+dx(w)),(dz(v)+dy(w))] //

macro GammaNL(u1,v1,w1,u2,v2,w2) [(dx(u1)*dx(u2)+dx(v1)*dx(v2)+dx(w1)*dx(w2))*0.5,
(dy(u1)*dy(u2)+dy(v1)*dy(v2)+dy(w1)*dy(w2))*0.5,  (dz(u1)*dz(u2)+dz(v1)*dz(v2)+dz(w1)*dz(w2))*0.5,
(dy(u1)*dx(u2)+dx(u1)*dy(u2)+dy(v1)*dx(v2)   +dx(v1)*dy(v2)+dy(w1)*dx(w2)+dx(w1)*dy(w2))*0.5,
(dz(u1)*dx(u2)+dx(u1)*dz(u2)+dz(v1)*dx(v2)   +dx(v1)*dz(v2)+dz(w1)*dx(w2)+dx(w1)*dz(w2))*0.5,
(dz(u1)*dy(u2)+dy(u1)*dz(u2)+dz(v1)*dy(v2)   +dy(v1)*dz(v2)+dz(w1)*dy(w2)+dy(w1)*dz(w2))*0.5] //

macro Gamma(u,v,w) (GammaL(u,v,w)+GammaNL(u,v,w,u,v,w)) //

macro dGammaNL(u,v,w,uu,vv,ww) (2.0*GammaNL(u,v,w,uu,vv,ww)) //

macro dGamma(u,v,w,uu,vv,ww) (GammaL(uu,vv,ww)+dGammaNL(u,v,w,uu,vv,ww)) //
```

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Implementation of the ANM for solid mechanics in FreeFem++

- P2 Lagrange FEM interpolation is assumed and defined on the mesh Th3D (tetrahedrons) via the command:

```
fespace Vh(Th3D,[P2,P2,P2]);
```

- The displacement field at each ANM order is declared:

```
Vh[int] [u,v,w](Norder+1);
```

- The command varf facilitates the computation of the tangent matrix, and the linear right-hand side:

```
varf PbTg ([u1,v1,w1],[uu,vv,ww]) =   int3d(Th3D) (
(dGamma(u[0],v[0],w[0],uu,vv,ww))'(D(GammaL(u1,v1,w1)+2*GammaNL(u[0],v[0],w[0],u1,v1,w1)))
+(dGammaNL(u1,v1,w1,uu,vv,ww))'*(D*(GammaL(u[0],v[0],w[0])+GammaNL(u[0],v[0],w[0],u[0],v[0],w
[0]))) )  + on(lencasmid,u1=0.,v1=0.,w1=0.);

varf PbF ([u1,v1,w1],[uu,vv,ww]) = int2d(Th3D,lrigthmid) (Pa*ww) +on(lencasmid,u1=0.,v1=0.,w1=0.);
```

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Implementation of the ANM for solid mechanics in FreeFem++

- In order to assemble the nonlinear right-hand side vector $\left\{ \mathrm{F}_2^{\mathrm{nl}} \right\}$, we define intermediate tensors $\left\{ \mathrm{S}_1 \right\}$ and $\left\{ \mathrm{S}_2^{\mathrm{nl}} \right\}$, written in vectorial form and defined at the Gauss points

```
fespace QFh6(ThL3D,[FEQF53d,FEQF53d,FEQF53d,FEQF53d,FEQF53d,FEQF53d]);
QFh6[int][Sxx,Syy,Szz,deuxSxy,deuxSxz,deuxSyz](Norder+1);
QFh6[Snlxx,Snlyy,Snlzz,deuxSnlxy,deuxSnlxz,deuxSnlyz](Norder+1);

[Sxx[1],Syy[1],Szz[1],deuxSxy[1],deuxSxz[1],deuxSyz[1]] =
DL*(GammaL(u[1],v[1],w[1])+2*GammaNL(u[0],v[0],w[0],u[1],v[1],w[1]));

[Snlxx,Snlyy,Snlzz,deuxSnlxy,deuxSnlxz,deuxSnlyz] = DL*(GammaNL(u[1],v[1],w[1],u[1],v[1],w[1]));

varf PbFnl2 ([u1,v1,w1],[uuu,vvv,www]) =  - int3d(Th3D) (
(dGammaNL(u[1],v[1],w[1],uuu,vvv,www))'*([Sxx[1],Syy[1],Szz[1],deuxSxy[1],deuxSxz[1],deuxSyz[1]])+
(dGamma(u[0],v[0],w[0],uuu,vvv,www))'*([Snlxx,Snlyy,Snlzz,deuxSnlxy,deuxSnlxz,deuxSnlyz]) )+
on(lencasmid,u1=0.,v1=0.,w1=0.);

Fnlu[]=PbFnl2(0,Vh);
```

- Equivalent commands are used at order $p \geq 2$

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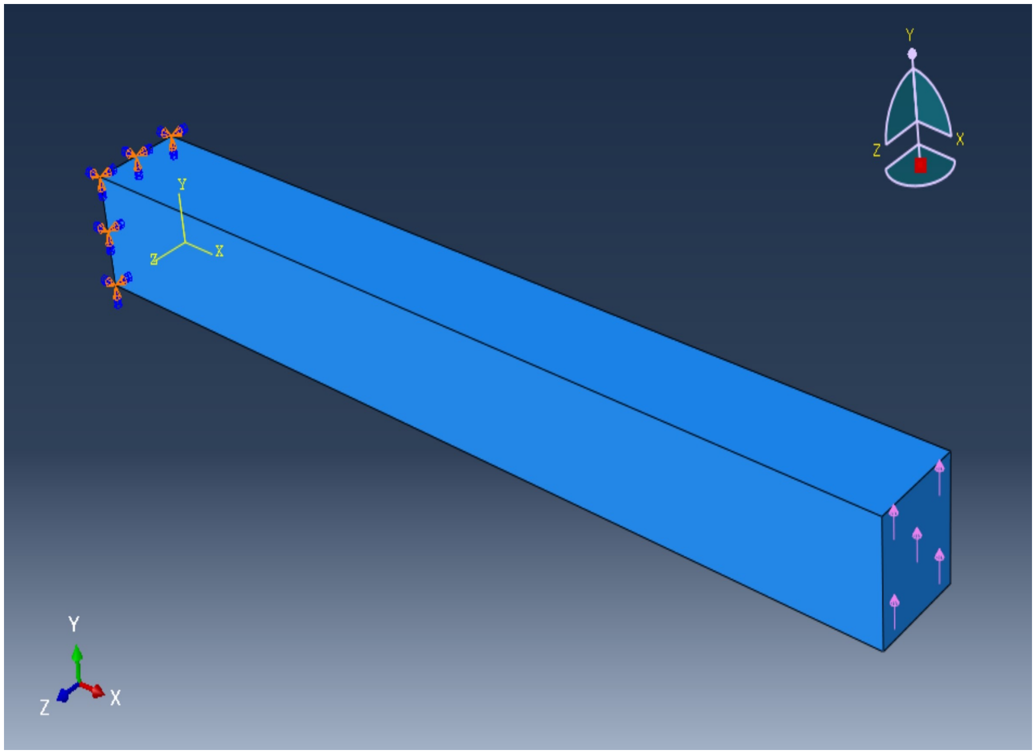
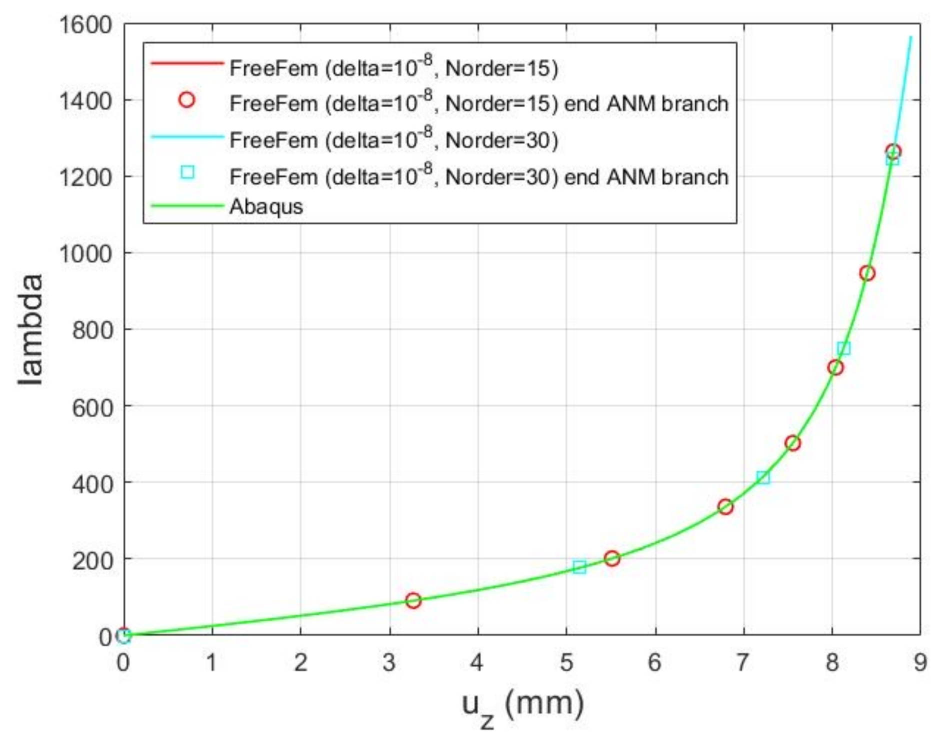
Numerical results

- Validation example: clamped beam subjected to a conservative vertical surface traction





Length: 10 mm, width and thickness 1 mm

Young's modulus 10^5 Mpa, Poisson's ratio 0.

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Numerical results

- Film-substrate system under axial compression: the film-substrate system being studied consists of a stiff film deposited on a soft rectangle parallelepiped substrate. It has already been studied with the help of ANM using a coupled between shell finite element and hexahedron finite elements by Fan Xu et al [4].

[4] F. Xu, M. Potier-Ferry, S. Bellouettar, Y. Cong, 3D finite element modeling for instabilities in thin films on soft substrate, International of Solids and Structures 51 (2014) 3619-3632.

- Geometrical nonlinear elasticity is assumed for the stiff film, and linear elasticity for the soft substrate.

- Young's modulus and Poisson's coeffcient of the substrate (1.8 Mpa, 0.48), and of the film (1.3×10^5 Mpa, 0.3).

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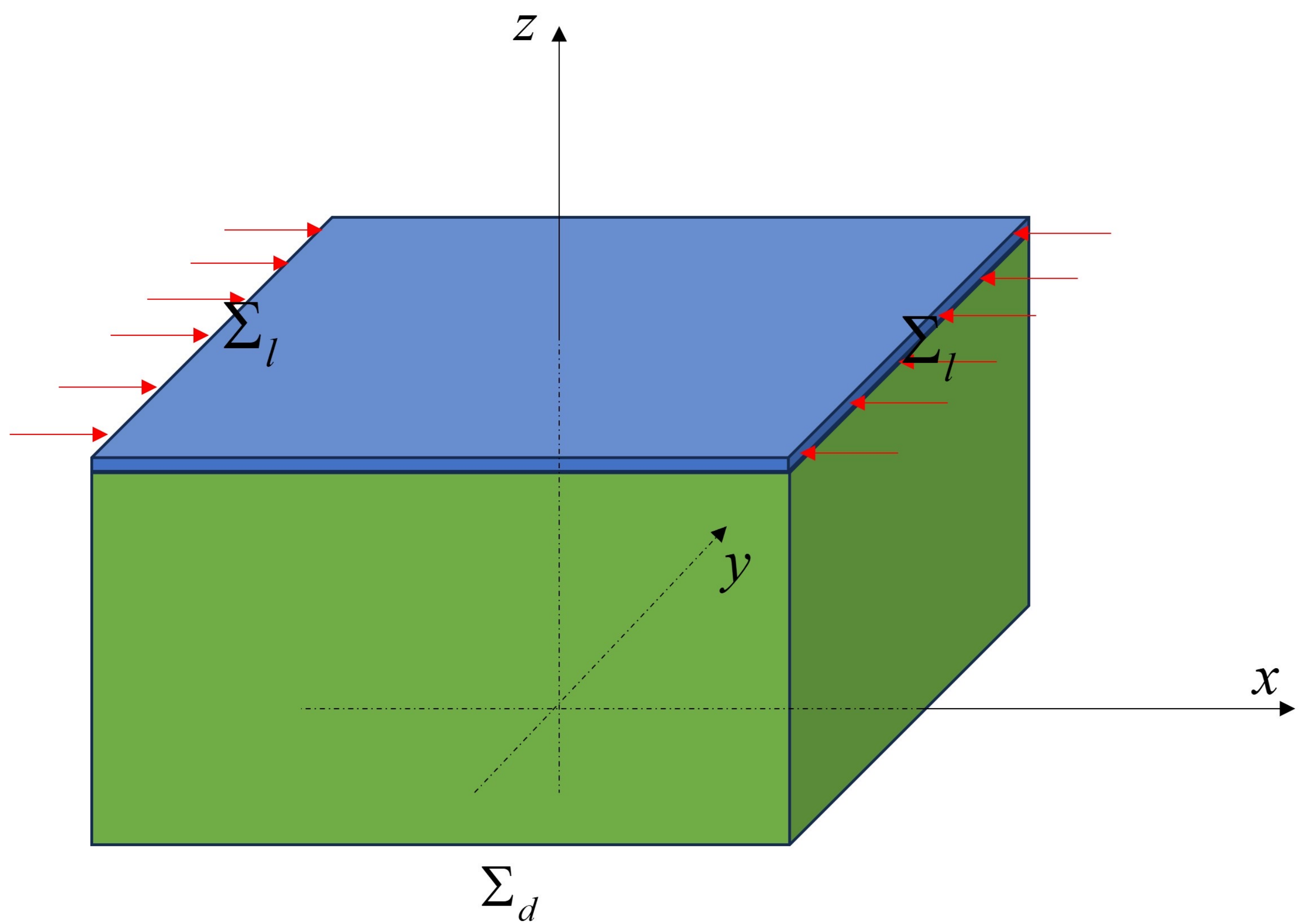
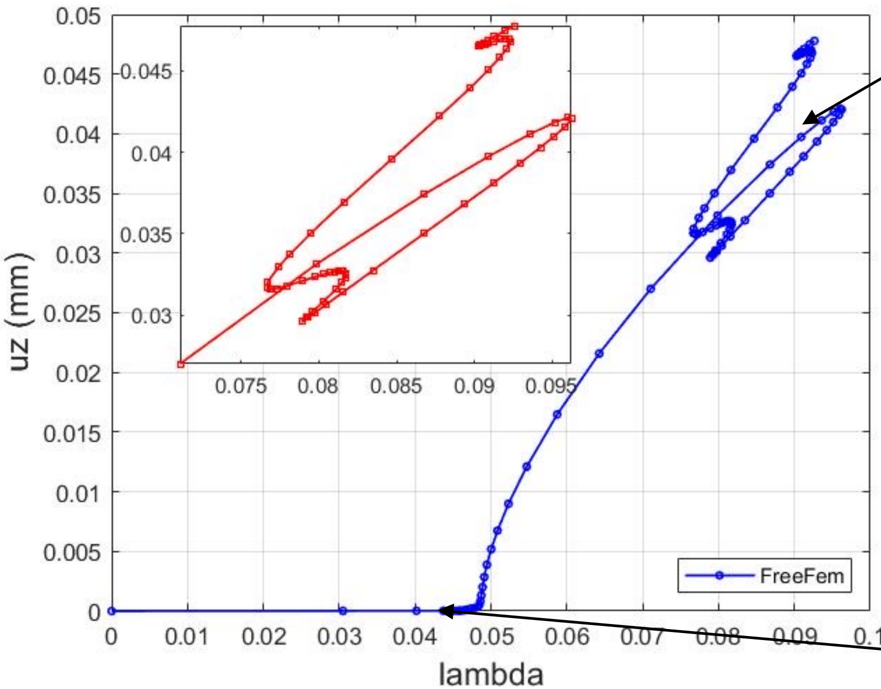
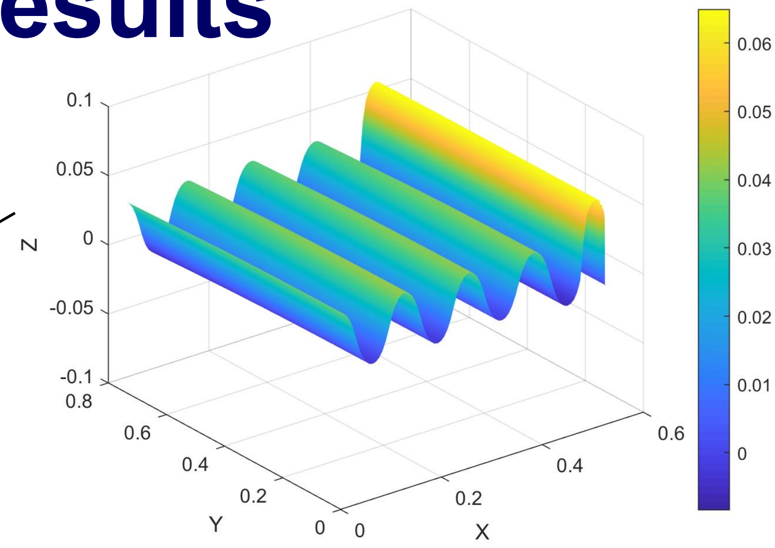
Numerical results

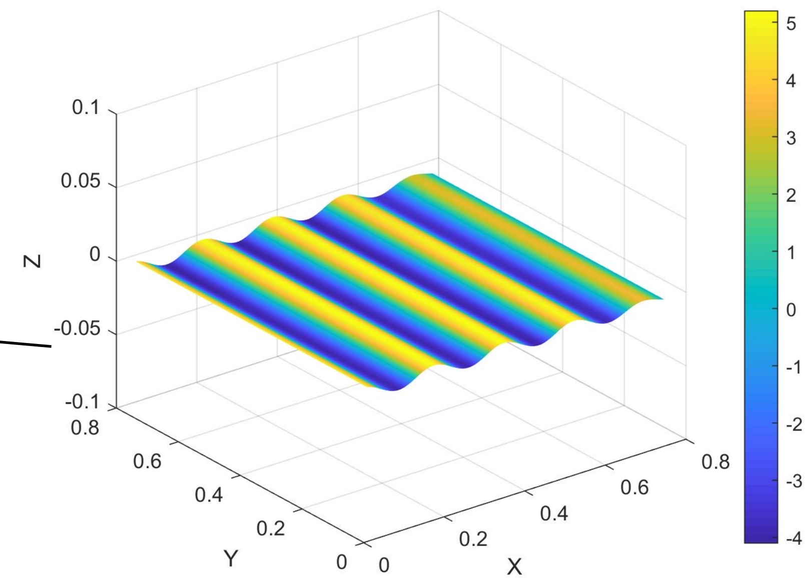
- Film-substrate system under axial compression



Numerical results







Bifurcation diagram: vertical displacement of the center of the film-substrate system (top surface) with $E_f / E_s = 0.72.10^5$

Numerical results

- Spherical film-substrate system under thermal loading: thermo-mechanical shrinkage of its compliant core.
- Xu et al. [5] have presented an analytical model, experimental, and numerical results. The numerical results have been obtained with the commercial software ABAQUS using both the Riks method and the pseudo dynamix method.

[5] F. Xu, S. Zhao, L. Conghua, M. Potier-Ferry, Pattern selection in core-shell spheres, Journal of the Mechanics and Physics of Solids 137 (2020) 103892.

- The relevant parameter to characterize surface morphological pattern formation of core-shell spheres upon shrinkage of core is

Substrate Young modulus

Film Young modulus

$$C_s = \left(\frac{E_s}{E_f}\right)\left(\frac{R}{h_f}\right)^{\frac{3}{2}}$$

Sphere radius

Film thickness

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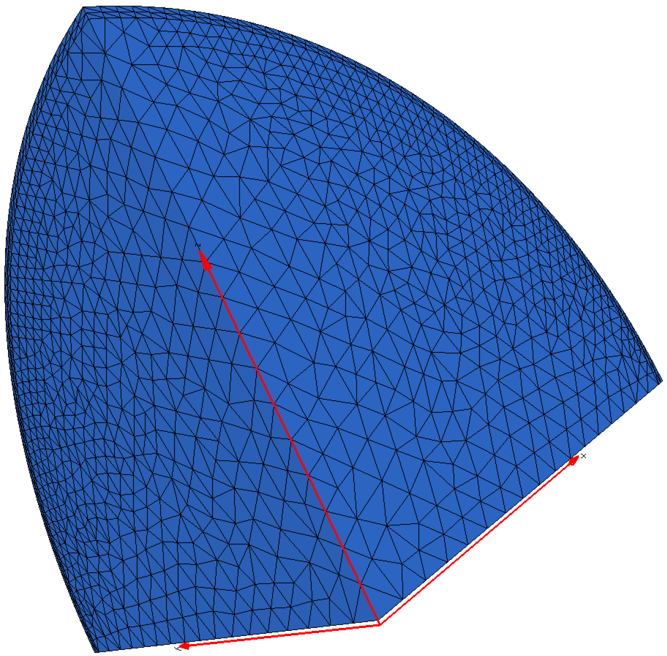
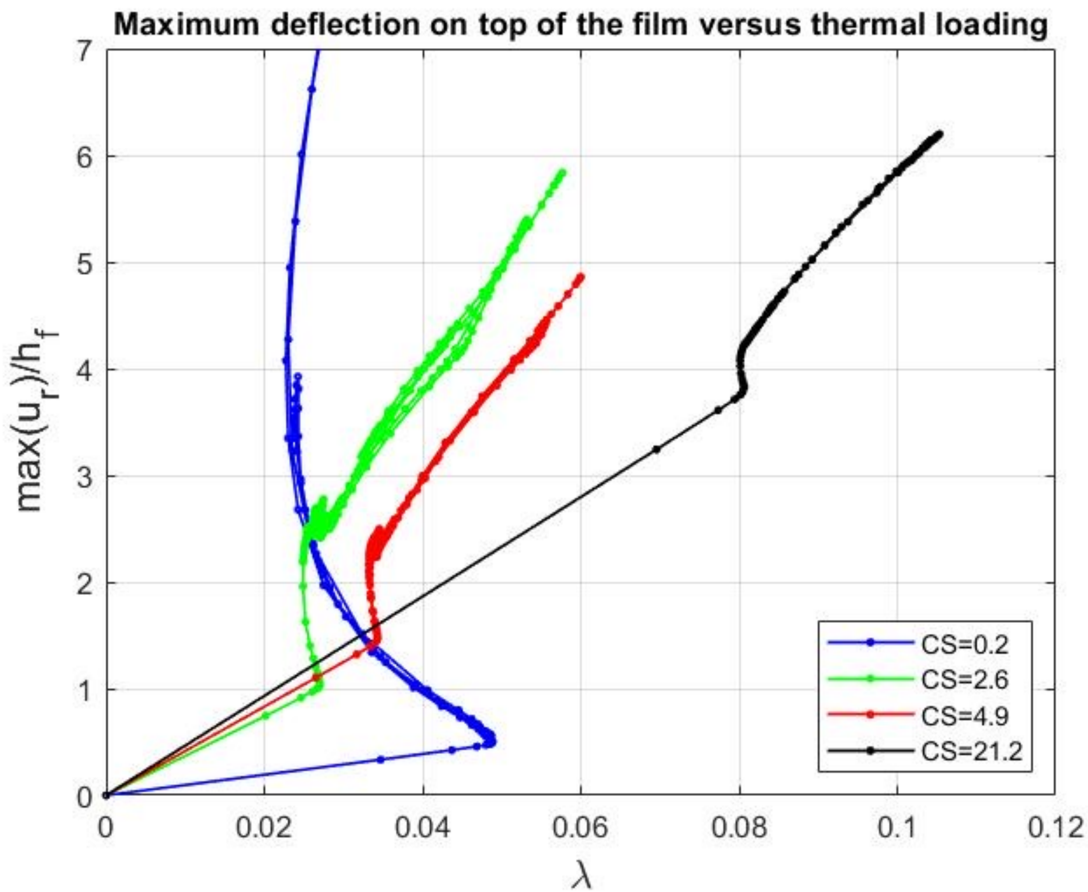
Numerical results



Tetrahedron mesh (1/8th sphere)



Bifurcation diagram for various Cs parameters

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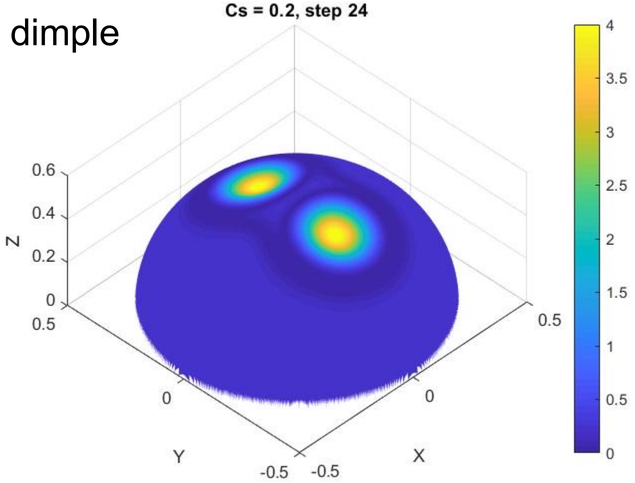
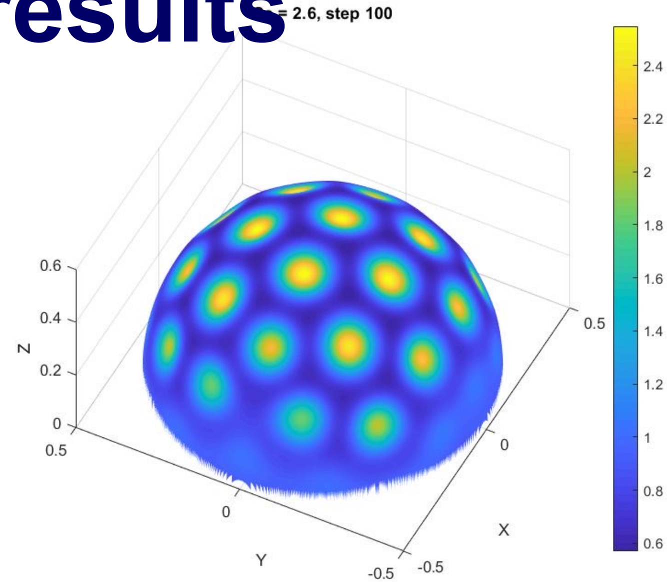
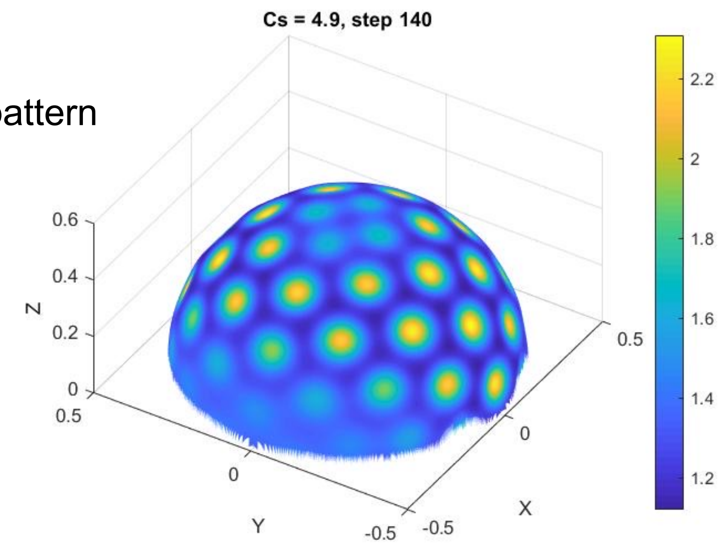
Numerical results

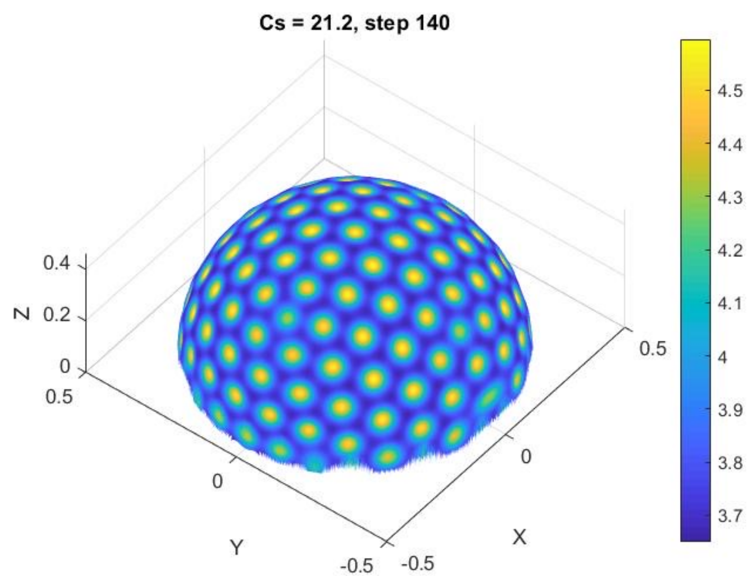
Isolated dimple





Bucky ball pattern





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Conclusions

- We have presented a new implementation of the Asymptotic Numerical Method within the user-friendly finite element environment FreeFem++. ANM continuation method, based on a perturbation technique, has proven to be a very efficient technique for the numerical simulation of nonlinear instability problems.

- Its high level Design Specific Language dedicated to variational formulations and finite elements makes it easier to write scripts for solving nonlinear solid or fluid mechanics problems using ANM. It will be very helpful for new developments.

- A first computation using the new developed FreeFem++ code, consisting in a cantilever (Saint Venant-Kirchhoff material) submitted to a vertical surface force, where geometrical nonlinearities are taken into account, has shown a very good comparison with the commercial software Abaqus.

- The two other applications concern film/substrate systems. The first case is the study of a planar film/substrate system subjected to axial compression, and the second case is a spherical film/substrate system subjected to the thermo-mechanical shrinkage of its core.

- Both film/substrate applications have demonstrated the efficiency of the implementation of ANM in FreeFem++ for the following of equilibrium paths when solving solid mechanical problems.

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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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