# Non linear mechanical simulation of thin films on soft substrate in the FreeFem++ environment


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# Outlines

- Introduction
- Asymptotic Numerical Method
- Application of the ANM to the non linear mechanical study of stiff thin films on soft substrates
- 3D implementation in the FreeFem++ environment
- Numerical results
- Conclusions

# Introduction

- Wrinkles of stiff thin layers on soft materials
  - Wrinkles in nature:

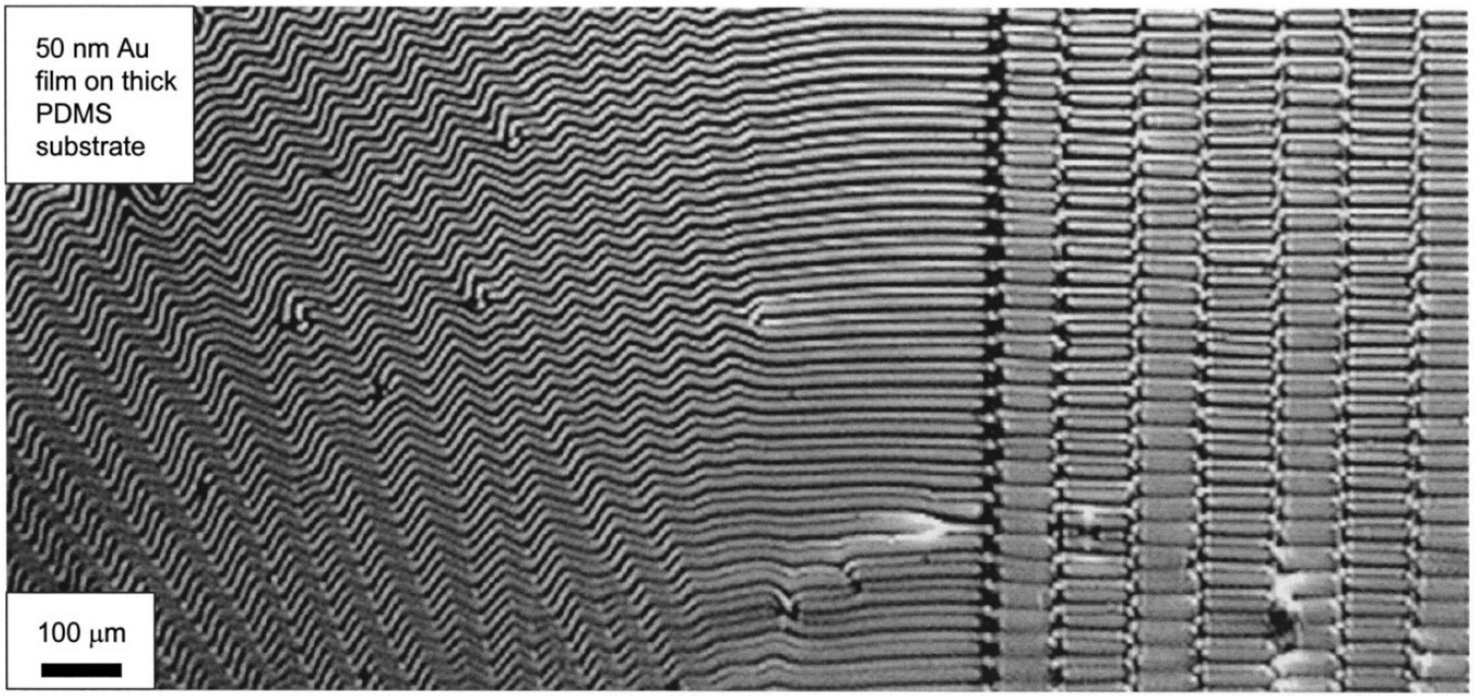
leaf

Human finger

Land form

# Introduction

- Buckling of a 50 nm gold film on a thick PDMS substrate



# Introduction

- Non linear mechanical problems are generally solved using predictor-corrector algorithms such as Newton Raphson scheme (Riks, 1972, 1984), (Ramm, 1981), ...

- A family of Asymptotic-Numerical-Method based on Taylor series and Finite Element Method has been developed for non linear elastic structures

  - Damil and Potier-Ferry (1990), compute perturbed bifurcations
  - Azrar, Cochelin, Damil, Potier-Ferry (1993), compute the post-buckling behavior of elastic plate
  - Cochelin, Damil, Potier-Ferry (1995), show the extension to any non linear elastic solutions

# Asymptotic Numerical Method (ANM)

- Consider the non linear problem :

(1)
$$\mathbf{R}(\mathbf{U},\lambda) = \mathbf{L}(\mathbf{U}) + \mathbf{Q}(\mathbf{U},\mathbf{U}) - \lambda\mathbf{F} = \mathbf{0}$$

Linear operator

Control parameter

Unknown vector

Quadratic operator

Vector

- Principles of the ANM : from a known solution $\left(\mathbf{U}^j,\lambda^j\right)$, the new solution is expanded into truncated power serie of a perturbation parameter a :

(2)
$$\begin{cases} \mathbf{U}(a) = \mathbf{U}^j + \sum_{p=1}^{N} a^p \mathbf{U}_p \\ \lambda(a) = \lambda^j + \sum_{p=1}^{N} a^p \lambda_p \end{cases}$$

# Asymptotic Numerical Method (ANM)

- A good choice for the parameter a is the linearized arc-length parameter defined by the projection of the pair $\left(\mathbf{U}-\mathbf{U}^j, \lambda-\lambda^j\right)$ on the tangent direction $\left(\mathbf{U}_1, \lambda_1\right)$

$$a = \left\langle \mathbf{U}-\mathbf{U}^j, \mathbf{U}_1 \right\rangle + \left(\lambda-\lambda^j\right)\lambda_1 \tag{3}$$

- By estimating the radius of convergence of the series, the validity range of a for each branch is:

$$a_{\max} = \left(\delta \frac{\|U_1\|}{\|U_N\|}\right)^{\frac{1}{N-1}} \tag{4}$$

- Truncation order: $15 \le N \le 50$ (5)

- tolerance $\delta$ (affects the residual): $10^{-6} \le \delta \le 10^{-3}$ (6)

# Asymptotic Numerical Method (ANM)

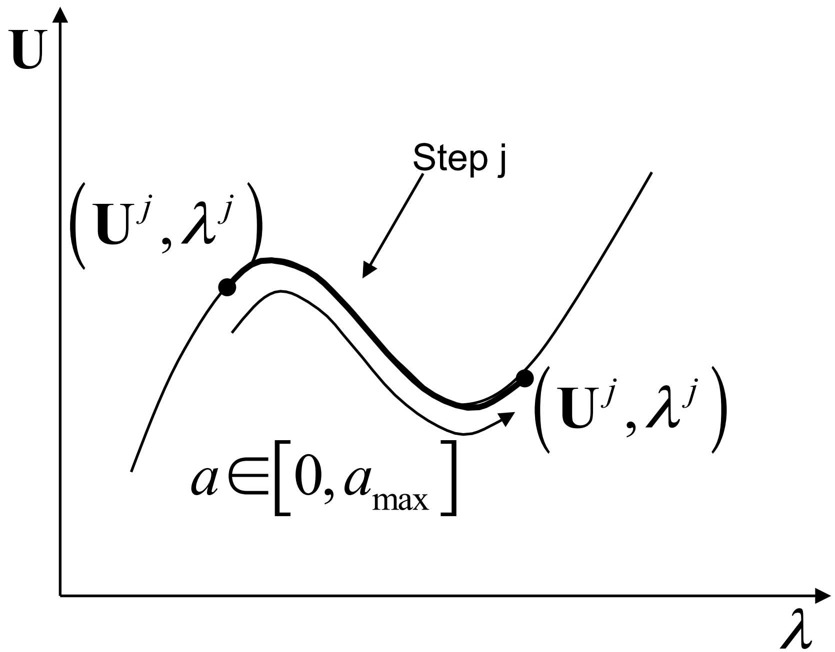
- By substituting (2) into (1) and (3), and equating terms with the same power of a, we obtain the following sequence of linear problems:

  - order 1: $L_t\left(\mathbf{U}_1\right)=\lambda_1\mathbf{F}$ , and, $\left\langle \mathbf{U}_1,\mathbf{U}_1\right\rangle+\lambda_1\lambda_1=1$ (7)
  - order 2: $L_t\left(\mathbf{U}_2\right)=\lambda_2\mathbf{F}-\mathbf{Q}\left(\mathbf{U}_1,\mathbf{U}_1\right)$, and, $\left\langle \mathbf{U}_2,\mathbf{U}_1\right\rangle+\lambda_2\lambda_1=0$ (8)

    $\vdots$
  - order p: $L_t\left(\mathbf{U}_p\right)=\lambda_p\mathbf{F}-\sum_{r=1}^{p-1}\mathbf{Q}\left(\mathbf{U}_r,\mathbf{U}_{p-r}\right)$, and, $\left\langle \mathbf{U}_p,\mathbf{U}_1\right\rangle+\lambda_p\lambda_1=0$ (9)

  With, the tangent operator $\mathbf{L}_t\left(.\right)$ defined by $\mathbf{L}_t\left(.\right)=\mathbf{L}\left(.\right)+2\mathbf{Q}\left(.,\mathbf{U}^j\right)$

# Asymptotic Numerical Method (ANM)

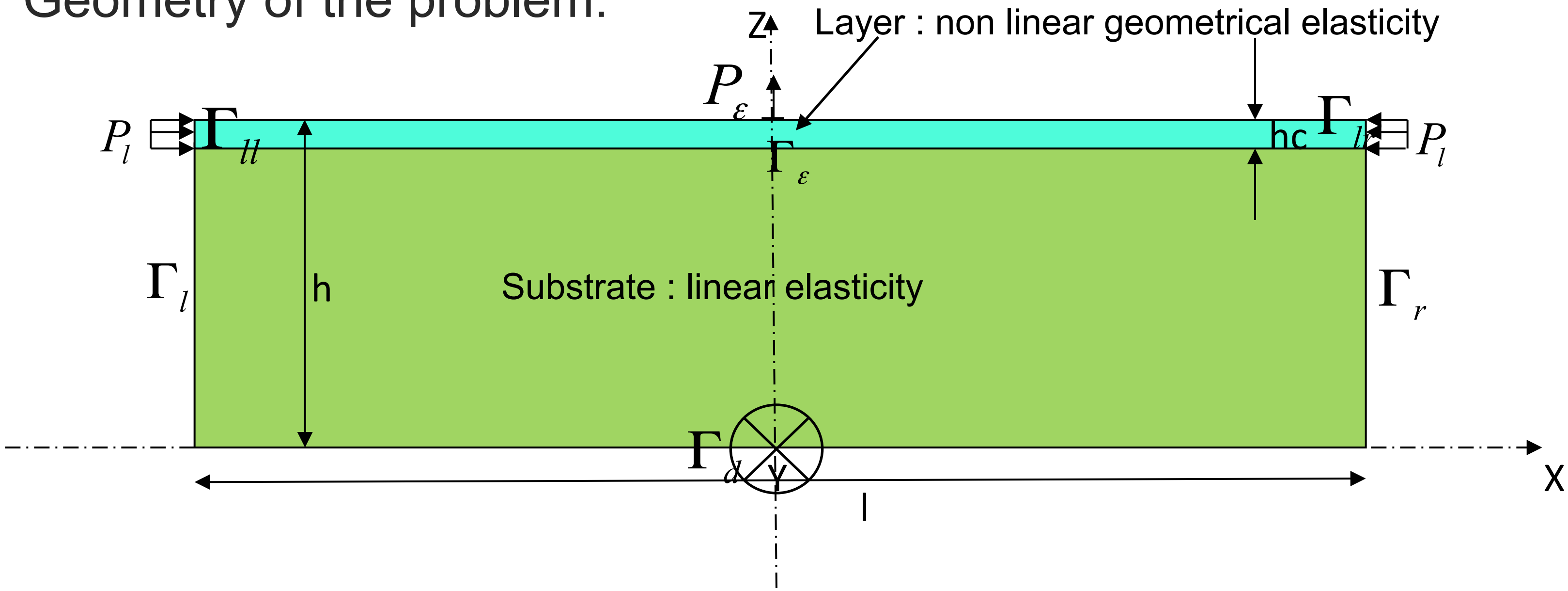



In case of bifurcation points:

▶ accumulation of small steps indicates the presence of a bifurcation

# Application of ANM to the non linear mechanical study of thin films on soft substrate

- Geometry of the problem:




- Elastic coefficients:
  - Substrate: $E_s = 1.8$ MPa, $\nu_s = 0.48$
  - Layer: $E_l = 1.3 \cdot 10^5$ MPa $\nu_l = 0.3$
- Boundary conditions: on $\Gamma_l, \Gamma_{ll}, \Gamma_r, \Gamma_{rl}$, $u_Y = u_Z = 0$, on $\Gamma_d$ $u_Z = 0$

  only model half structure, symmetry with respect to the (x=0) plane

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- Assumptions for the mechanical model ($E_L \gg E_S$)
  - Non linear geometrical elasticity in the layer
  - Linear elasticity in the substrate
- Instabilities appear for small deformations
- Fan Xu's PhD thesis Dec 2014 : "numerical study of instability patterns of film substrate patterns", based on a plate finite element formulation for the film.

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- For elastic bodies, the governing equations can be stated from the mixed Hellinger-Reissner functional.

Green-Lagrange strain tensor

$$HR(\mathbf{u},\mathbf{S},\lambda) = \int_\Omega \left( \mathbf{S} : \gamma - \frac{1}{2} \mathbf{S} : \mathbf{D}^{-1} : \mathbf{S} \right) d\Omega - \lambda P_e(\mathbf{u}) \qquad (10)$$

Elasticity matrix

Piola-Kirchhoff stress tensor of the second kind

with,
$$P_e(\mathbf{u}) = -\int_{\Gamma_{lr}} P_l u_x + \int_{\Gamma_{ll}} P_l u_x + \int_{\Gamma_\varepsilon} P_\varepsilon u_z \qquad (11)$$

Small perturbed force

Lateral surface forces

- Let us compute the variational formulation:

$$\int_\Omega \left( \mathbf{S} : \delta\gamma + \delta\mathbf{S} : \gamma - \mathbf{S} : \mathbf{D}^{-1} : \delta\mathbf{S} \right) d\Omega - \lambda P_e(\delta\mathbf{u}) = 0 \qquad (12)$$

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- The Green Lagrange tensor is:

$$\gamma(\mathbf{u}) = \underbrace{\frac{1}{2}\left(\nabla\mathbf{u} + \nabla^T\mathbf{u}\right)}_{\gamma_l(\mathbf{u})} + \underbrace{\frac{1}{2}\left(\nabla^T\mathbf{u}\cdot\nabla\mathbf{u}\right)}_{\gamma_{nl}(\mathbf{u},\mathbf{u})} = \gamma_l(\mathbf{u}) + \gamma_{nl}(\mathbf{u},\mathbf{u}) \qquad (13)$$

which gives:

$$\delta\gamma = \gamma_l(\delta\mathbf{u}) + \underbrace{2\gamma_{nl}(\mathbf{u},\delta\mathbf{u})}_{\delta\gamma_{nl}(\mathbf{u},\delta\mathbf{u})} = \gamma_l(\delta\mathbf{u}) + \delta\gamma_{nl}(\mathbf{u},\delta\mathbf{u}) \qquad (14)$$

- The serial developments of the ANM leads to:

$$\begin{cases} \mathbf{u}(a) = \mathbf{u}^j + \sum_{p=1}^{N} a^p \mathbf{u}_p \\ \lambda(a) = \lambda^j + \sum_{p=1}^{N} a^p \lambda_p \end{cases} \qquad (15)$$

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- By introducing (15) into (12), by identifying the order p terms, we obtain the following variational formulation:

$$\begin{aligned}
&\int_\Omega \delta\gamma^T\left(\mathbf{u}^j,\delta\mathbf{u}\right)\mathbf{D}\left(\gamma_l\left(\mathbf{u}_p\right)+2\gamma_{nl}\left(\mathbf{u}^j,\mathbf{u}_p\right)\right)d\Omega+\int_\Omega \delta\gamma_{nl}^T\left(\mathbf{u}_p,\delta\mathbf{u}\right)\mathbf{D}\left(\gamma_l\left(\mathbf{u}^j\right)+2\gamma_{nl}\left(\mathbf{u}^j,\mathbf{u}^j\right)\right)d\Omega \\
&-\lambda_p P_e\left(\delta\mathbf{u}\right)+\sum_{r=1}^{p-1}\int_\Omega \delta\gamma_{nl}^T\left(\mathbf{u}_{p-r},\delta\mathbf{u}\right)\mathbf{D}\left(\gamma_l\left(\mathbf{u}_r\right)+2\gamma_{nl}\left(\mathbf{u}^j,\mathbf{u}_r\right)+\sum_{s=1}^{r-1}\gamma_{nl}\left(\mathbf{u}_{r-s},\mathbf{u}_s\right)\right) \\
&+\int_\Omega \delta\gamma^T\left(\mathbf{u}^j,\delta\mathbf{u}\right)\mathbf{D}\left(\sum_{r=1}^{p-1}\gamma_{nl}\left(\mathbf{u}_{p-r},\mathbf{u}_r\right)\right)d\Omega=0
\end{aligned} \qquad (16)$$

- For the first order, the resulting variational formulation is:

$$\begin{aligned}
&\int_\Omega \delta\gamma^T\left(\mathbf{u}^j,\boldsymbol{\delta}\mathbf{u}\right)\mathbf{D}\left[\gamma_l\left(\mathbf{u}_1\right)+2\gamma_{nl}\left(\mathbf{u}^j,\mathbf{u}_1\right)\right]d\Omega \\
&+\int_\Omega \delta\gamma_{nl}{}^T\left(\mathbf{u}_1,\boldsymbol{\delta}\mathbf{u}\right)\mathbf{D}\left[\gamma_l\left(\mathbf{u}^j\right)+2\gamma_{nl}\left(\mathbf{u}^j,\mathbf{u}^j\right)\right]d\Omega-\lambda_1 P_e\left(\delta\mathbf{u}\right)=0
\end{aligned} \qquad (17)$$

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- P2 finite element model is used which leads to the linear systems: (for each branch).

  - Order 1: $\left[\mathbf{K}_T\right]\hat{\mathbf{U}}_1 = \mathbf{F}$

$$\begin{cases} \lambda_1 = \dfrac{1}{\sqrt{1+\hat{\mathbf{U}}_1{}^T\hat{\mathbf{U}}_1}} \\ \mathbf{U}_1 = \lambda_1\hat{\mathbf{U}}_1 \end{cases}$$

  - Order 2: $\left[\mathbf{K}_T\right]\mathbf{U}_2 = \lambda_2\mathbf{F} + \mathbf{F}_2^{nl} \quad \left(\mathbf{F}_2^{nl} \text{ computed using } \mathbf{U}_1\right)$

$$\begin{cases} \lambda_2 = -\lambda_1\left(\mathbf{U}_2^{nl}\right)^T\mathbf{U}_1 \\ \mathbf{U}_2 = \dfrac{\lambda_2}{\lambda_1}\mathbf{U}_1 + \mathbf{U}_2^{nl} \end{cases} \qquad \text{with, } \mathbf{U}_2^{nl} = \left[\mathbf{K}_T\right]^{-1}\mathbf{F}_2^{nl}$$

# Application of ANM to the non linear mechanical study of stiff thin films on soft substrate

- Order p: $[\mathbf{K}_T]\mathbf{U}_p = \lambda_p \mathbf{F} + \mathbf{F}_p^{nl} \quad \left(\mathbf{F}_p^{nl} \text{ computed using } \mathbf{U}_1, \mathbf{U}_2, \ldots, \mathbf{U}_{p-1}\right)$

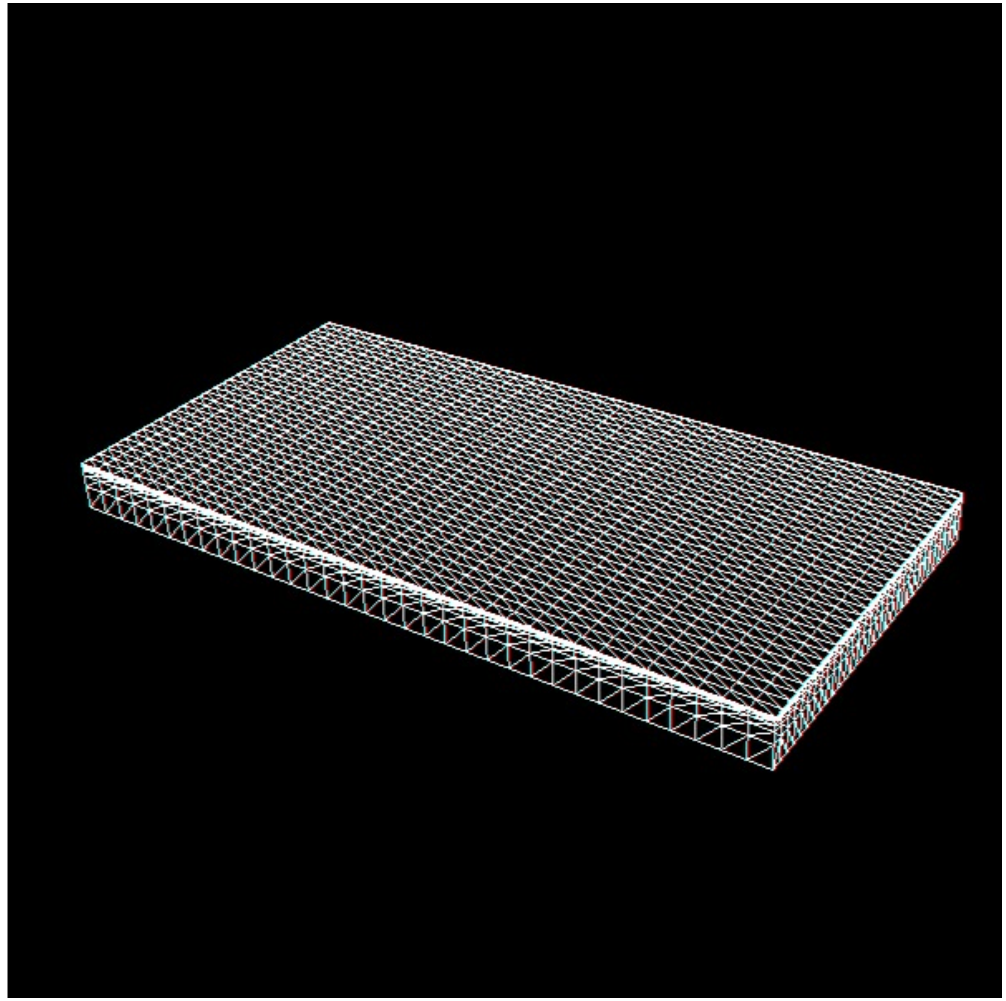
$$\begin{cases} \lambda_p = -\lambda_1 \left(\mathbf{U}_p^{nl}\right)^T \mathbf{U}_1 \\ \mathbf{U}_p = \dfrac{\lambda_p}{\lambda_1}\mathbf{U}_1 + \mathbf{U}_p^{nl} \end{cases} \qquad \text{with, } \mathbf{U}_p^{nl} = [\mathbf{K}_T]^{-1}\mathbf{F}_p^{nl}$$

The direction of the path in the branch is determined knowing the tangent of the displacement for the previous branch.

# 3D implementation in the FreeFem++ environment

- Main advantages of using FreeFem++:
  - use volume Finite Elements
  - powerful open source mathematical libraries are available
  - allows to compute problems with huge number of degrees of freedom by using parallel computing on HPC
  - allows to check stability of solutions

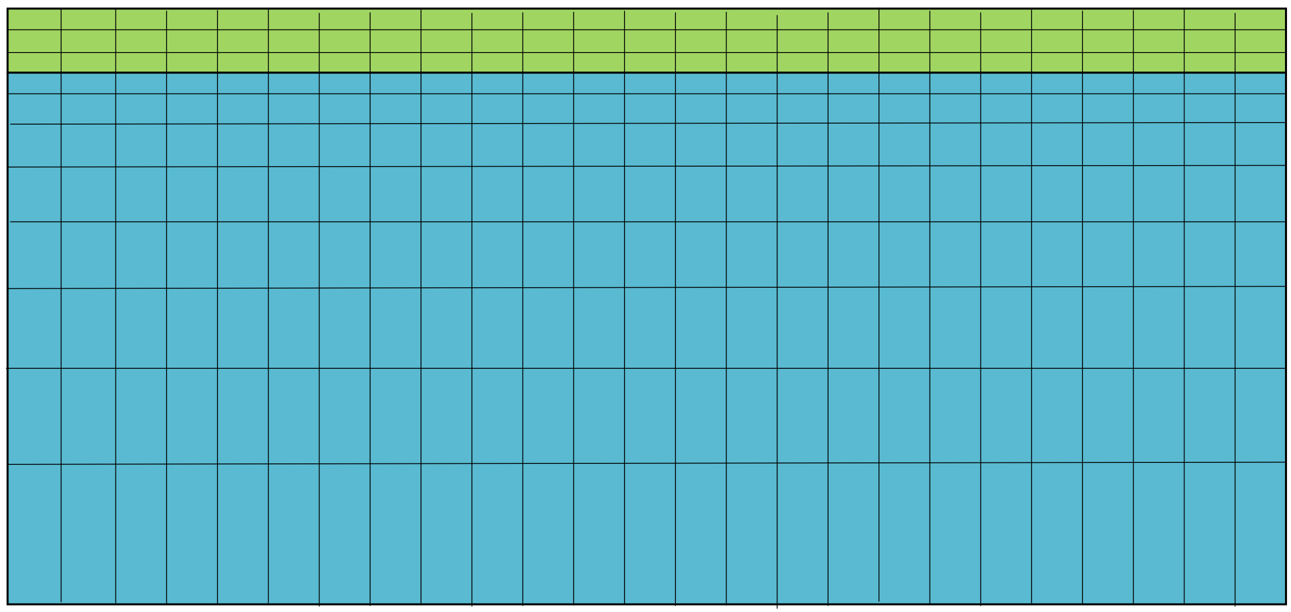
# 3D implementation in the FreeFem++ environment



- 3D Finite Element mesh
- Tetrahedral Finite Elements
- P2 quadratic Lagrangian interpolation
- Number of nodes: 187 005
- CPU time (almost 3 days)
- improvement with parallel programming

# 3D implementation in the FreeFem++ environment

- 3D mesh obtained from a 2D mesh
- 2D mesh: uniform mesh in the layer, geometrical rate in the substrate



# 3D implementation in the FreeFem++ environment

- Let us present the main features of the FreeFem++ code:
  - macro are used to define the Green Lagrange tensor and its differential:

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

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  ] // EOM


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

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

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

# 3D implementation in the FreeFem++ environment

- Definition of the finite element space

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

- Creation of the tangent matrix $\left[\mathbf{K}_T\right]$ and the second member $\mathbf{F}$

```
varf PbTg ([u1,v1,w1],[uu,vv,ww]) = int3d(Th3D,reg3DS) (  (GammaL(uu,vv,ww))'*(DS*(GammaL(u1,v1,w1)))  )
+ int3d(Th3D,reg3DL) (
        (dGamma(u[0],v[0],w[0],uu,vv,ww))'*(DL*(GammaL(u1,v1,w1)+2*GammaNL(u[0],v[0],w[0],u1,v1,w1)))
                                                                                              +
(dGammaNL(u1,v1,w1,uu,vv,ww))'*(DL*(GammaL(u[0],v[0],w[0])+GammaNL(u[0],v[0],w[0],u[0],v[0],w[0])))  )
        + int2d(Th3D,lrightlmid) ( Pa*uu ) + Force
        + on(lsymmid,u1=0.) + on(lrightmid,lrightlmid,v1=0.,w1=0.)+on(ldownmid,w1=0);

matrix Kt = PbTg(Vh,Vh,solver=sparsesolver);
Fu[] = PbTg(0,Vh);
```

# 3D implementation in the FreeFem++ environment

- Computation of $\mathbf{F}_2^{nl}$

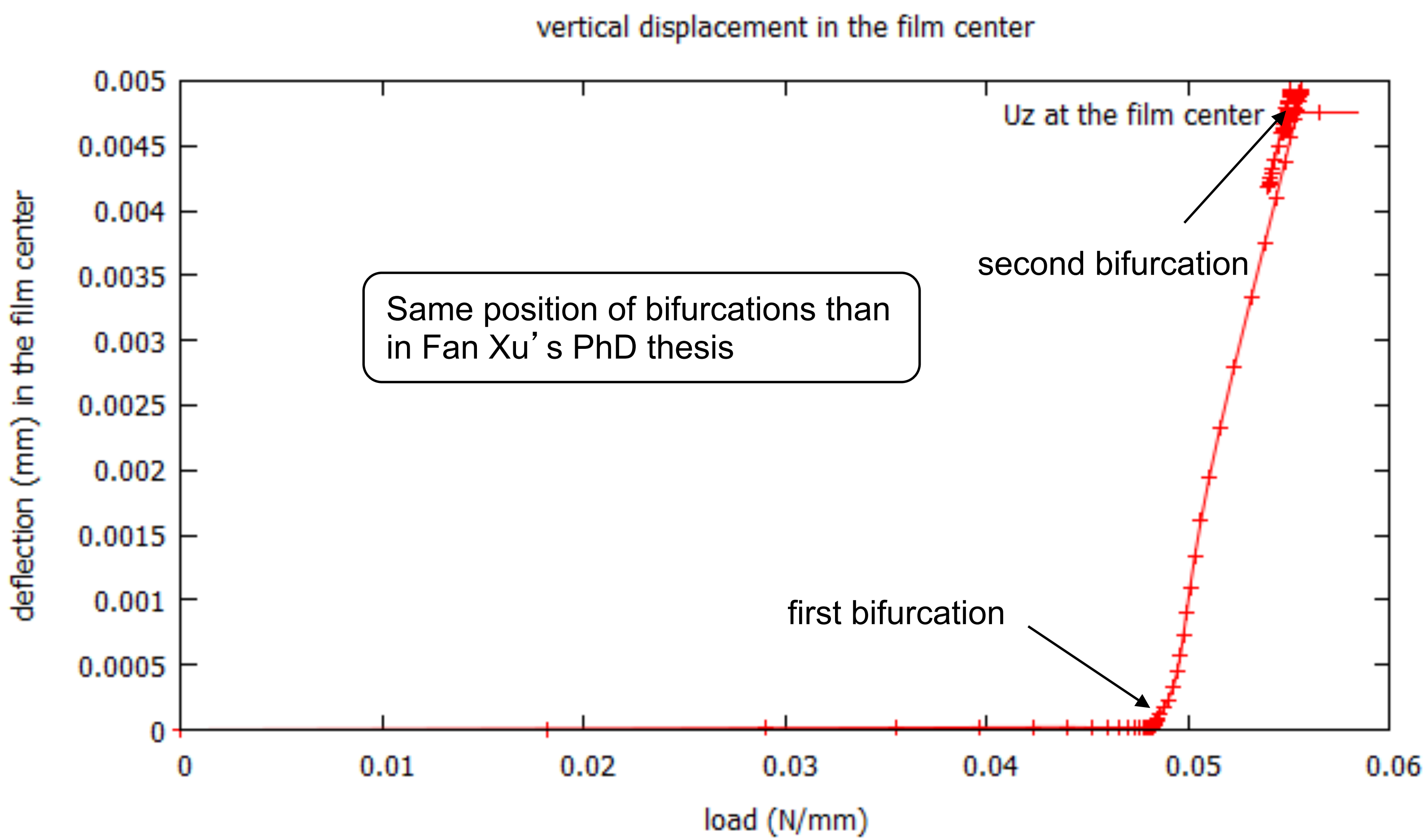
```
varf PbFnl2 ([utmp,vtmp,wtmp],[uuu,vvv,www]) =  - int3d(Th3D,reg3DL)
(   (dGammaNL(u[1],v[1],w[1],uuu,vvv,www))'*(DL*(GammaL(u[1],v[1],w[1])+2*GammaNL(u[0],v[0],w[0],u[1],v[1],w[1])))
+ (dGamma(u[0],v[0],w[0],uuu,vvv,www))'*(DL*(GammaNL(u[1],v[1],w[1],u[1],v[1],w[1]))) )

            + on(lsymmid,utmp=0.) + on(lrightmid,lrightlmid,vtmp=0.,wtmp=0.)+on(ldownmid,wtmp=0);

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

- Computation of $\mathbf{F}_p^{nl}$ for p>2 : double loop sum is needed

# 3D implementation in the FreeFem++ environment

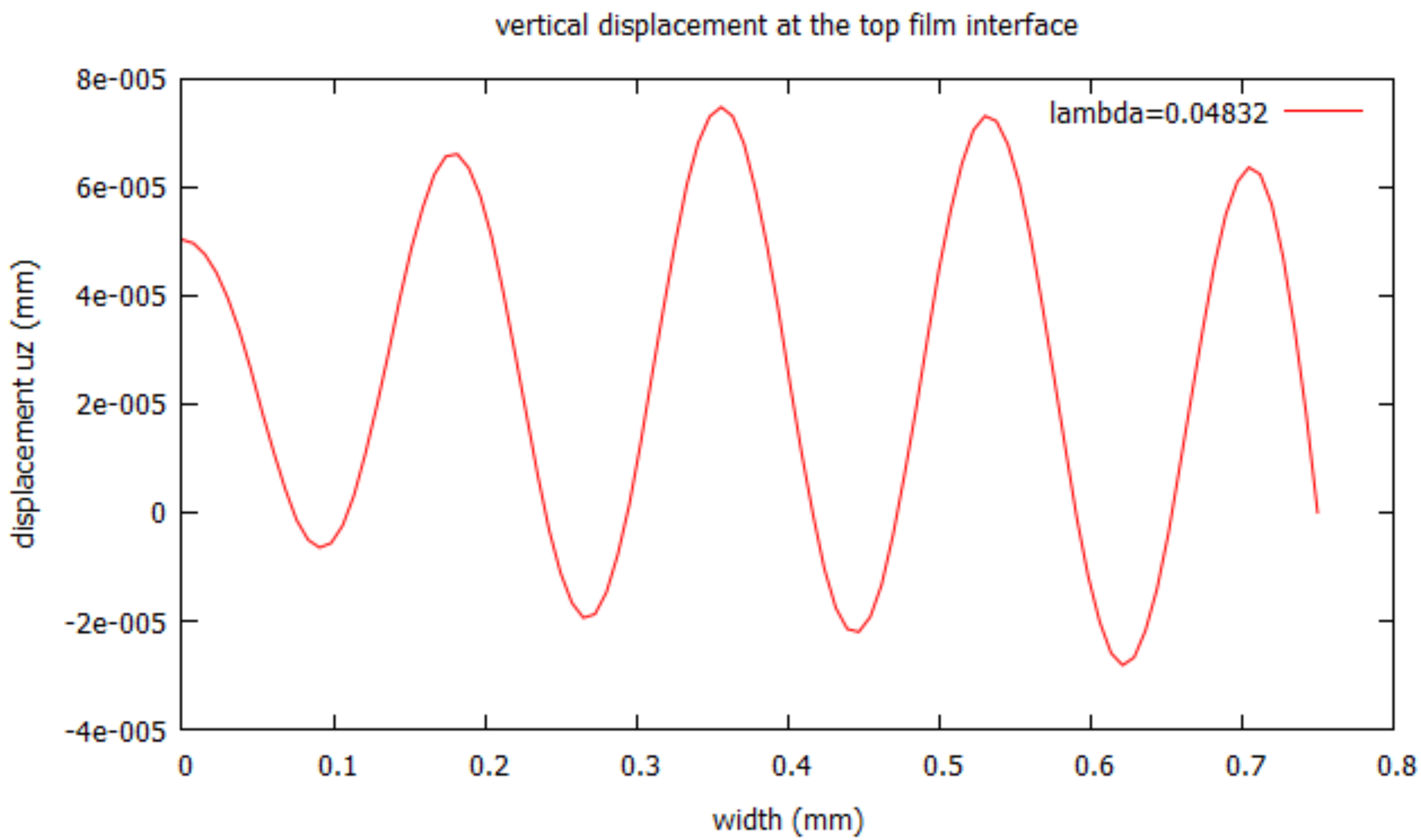
```
[Fnlu,Fnlv,Fnlw] = [0.,0.,0.];
for (int ir=1;ir<ipn;ir++)
{
   varf PbFnla ([utmp,vtmp,wtmp],[uuu,vvv,www]) = - int3d(Th3D,reg3DL) (  (dGammaNL(u[ipn-ir],v[ipn-ir],w[ipn-ir],uuu,vvv,www))'*(DL*(GammaL(u[ir],v[ir],w[ir])
+2*GammaNL(u[0],v[0],w[0],u[ir],v[ir],w[ir]))) );
   Fnlutmp[] = PbFnla(0,Vh);
   Fnlu[] = Fnlu[] + Fnlutmp[];
   for (int is=1;is<ir;is++)
   {
      varf PbFnlb([utmp,vtmp,wtmp],[uuu,vvv,www]) =  - int3d(Th3D,reg3DL) (  (dGammaNL(u[ipn-ir],v[ipn-ir],w[ipn-    ir],uuu,vvv,www))'*(DL*(GammaNL(u[ir-is],v[ir-
is],w[ir-is],u[is],v[is],w[is]))) );
      Fnlutmp[] = PbFnlb(0,Vh);

      Fnlu[] = Fnlu[] + Fnlutmp[];

   }
   varf PbFnlc ([utmp,vtmp,wtmp],[uuu,vvv,www]) =  - int3d(Th3D,reg3DL) (  (dGamma(u[0],v[0],w[0],uuu,vvv,www))'*(DL*(GammaNL(u[ipn-ir],v[ipn-ir],w[ipn-
ir],u[ir],v[ir],w[ir]))) );
    Fnlutmp[] = PbFnlc(0,Vh);
    Fnlu[] = Fnlu[] + Fnlutmp[];
}
varf PbFnlCL ([utmp,vtmp,wtmp],[uuu,vvv,www]) =  on(lsymmid,utmp=0.) + on(lrightmid,lrightlmid,vtmp=0.,wtmp=0.) + on(ldownmid,wtmp=0);
Fnlutmp[] = PbFnlCL(0,Vh);
Fnlu[] = Fnlu[] + Fnlutmp[];
```

# Numerical results




Bifurcation curve of the film / substrate under uniaxial compression

# Numerical results




Vertical displacement for $\lambda = 0.04832$ at the top film interface

# Conclusions

- it has been demonstrated that ANM can be used to study non linear problems
- the FreeFem++ numerical development tool is very efficient to implement the ANM algorithm of non linear mechanical problems
- it has been applied to simulate the non linear mechanical behavior of thin films on soft substrates
- both bifurcation curve and plot of the vertical displacement at the top interface have been shown
- the positions of the two first bifurcations are close to Fan Xu's results

# Thank you for your attention