Introduction to Modulef: simulation of a Quartz Crystal Microbalance displacement

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1 Definition of the structure

We define a 3D structure by first defining the 2D projection in the (X, Y) plane of the structure using `apnoxx`, and expand the third dimension using apn3xx. We will first focus on the definition of the 2D structure, and later develop the use of `apn3xx` which allows defining the properties of each surface/node of the final volume.

1.1 2D definition using `apnoxx`

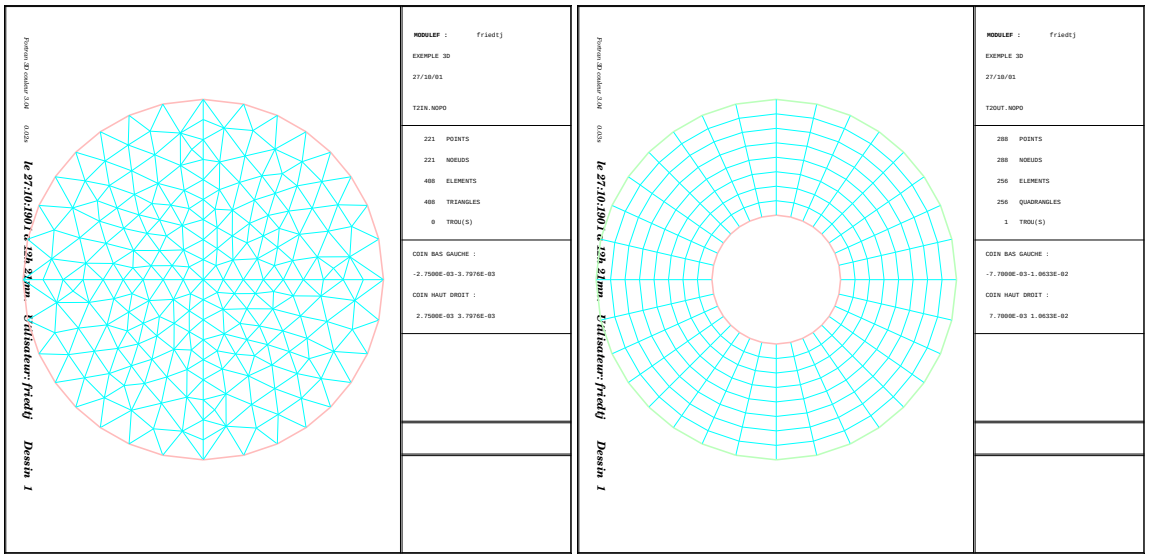

Figure 1: The two basic 2D structures required for defining the internal electrode coated part of the crystal and the external, non-coated part of the crystal resonator.

The two 2D structures developed for representing the QCM are presented here (figure 1). We have chosen to divide the QCM in two concentric circular pieces in order to be able to differentiate the gold coated counter electrode from the gold-free part of the QCM and hence simulate the effect of a finite sized electrode.

We first define one quarter (the bottom left) of the disc, rotate three times by 90^o and paste the resulting pieces in order to build the disc. We have chosen to rotate and paste the pieces in `apnoxx` rather than in `apn3xx` in order to be able to use the sub-domain and element numbering functions of the sub-processor `MA23` of `apn3xx` which would not have been available otherwise (since the rotation and gluing steps are made after the addition of the third dimension in `apn3xx`).

One difficulty comes from the fact that the two elementary pieces do not have the same number of sides, and thus require different mesh base elements and thus different finite elements. The inner element has an odd number of sides and requires a triangular mesh, while the outer element has an even number of sides and require a mesh element with 4 sides.

1.2 3D definition using `apn3xx`

Our choice in the number of sub-parts for creating the final volume and the order in which we join them together (using `apn3xx` rather than in `apnoxx`) results from our requirement of defining

```
'EXEMPLE 3D                                                    '
COURBES
     1                                  $ IMPRE
 COURBE01(X,Y)=
       X**2+Y**2-0.0025**2;
FIN
'POIN                                                          '
     1     3                            $ IMPRE NPOINT  $
$   NOP   NOREF(NOP)     X(NOP).           Y(NOP).  $
     1       1         0.000000E+00     0.000000E+00
     2       1         0.000000E+00     -.002500E+00
     3       1         0.002500E+00     0.000000E+00
'LIGN                                                          '
     1     3                            $ IMPRE  NDLM   $
$   NOLIG NOELIG NEXTR1 NEXTR2 NOREFL NFFRON       RAISON $
       1     10      1      2      0      0     0.100000E+01
       2      9      2      3      1     10     0.100000E+01    $ 5 -> 9
       3     10      3      1      0      0     0.100000E+01
'TRIH                                                          '
     1     0     1     3     1          $ IMPRE NIVEAU NUDSD NBRELI NS1L
 $ LISTE DES LIGNES DU CONTOUR :
     1     2     3
     1     0     1                            $ IMAX NQUAD
     3
```

```
'REGU                                                          '
     1     0     1
'ROTA                                                          '
     1     1     2                    $ IMPRE NIVEA1 NIVEA2
     0     0                          $ NBNNF NBNNSD
  0.90000E+02  0.00000E+00  0.00000E+00 $ TETA. X. Y.
'RECO'
     1     1     2     3  0.02000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS
     0     0                                              $ NBNNF NBNNSD
'ROTA                                                          '
     1     3     4                    $ IMPRE NIVEA1 NIVEA2
     0     0                          $ NBNNF NBNNSD
  0.18000E+03  0.00000E+00  0.00000E+00 $ TETA. X. Y.
'RECO'
     1     3     4     5  0.02000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS
     0     0                                              $ NBNNF NBNNSD
'RENC'
     1     5     6
'SAUV                                                          '
     1     6     0                    $ IMPRE NINOPO NTNOPO
 T2IN.NOPO
 $ NOM FICHIER
'FIN                                                           '
```

Table 1: The definition of the inner 2D structure (`T2INNOPO.DATA`)

```
'EXEMPLE 3D                                                    '
COURBES
     1                                  $ IMPRE
 COURBE01(X,Y)=
       X**2+Y**2-0.0025**2;
 COURBE02(X,Y)=
       X**2+Y**2-0.007**2;
FIN
'POIN                                                          '
     1     5                            $ IMPRE NPOINT  $
$   NOP   NOREF(NOP)     X(NOP).           Y(NOP).  $
     1       1         0.000000E+00     0.000000E+00
     2       1         0.000000E+00     -.002500E+00
     3       1         0.002500E+00     0.000000E+00
     4       2         0.000000E+00     -.0070000E+00
     5       2         0.007000E+00     0.000000E+00
'LIGN                                                          '
     1     7                            $ IMPRE  NDLM   $
$   NOLIG NOELIG NEXTR1 NEXTR2 NOREFL NFFRON       RAISON $
       1      4      1      2      1      0     0.100000E+01
       2      5      2      3      1     10     0.100000E+01
       3      4      3      1      1      0     0.100000E+01
       4      9      2      4      0      0     0.100000E+01   $ 5 -> 9
       5      9      4      5      2     10     0.100000E+01   $ 5 -> 9
       6      9      5      3      0      0     0.100000E+01   $ 5 -> 9
       7      9      2      3      1     10     0.100000E+01   $ 5 -> 9
```

```
'QUAC                                                          '
     1     2     2     4     1          $ IMPRE NIVEAU NUDSD NBRELI NS1L
 $ LISTE DES LIGNES DU CONTOUR :
     4     5     6     7
     9     1                                          $ 5 -> 9
'ROTA                                                          '
     1     2     3                    $ IMPRE NIVEA1 NIVEA2
     0     0                          $ NBNNF NBNNSD
  0.90000E+02  0.00000E+00  0.00000E+00 $ TETA. X. Y.
'RECO'
     1     2     3     4  0.02000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS
     0     0                                              $ NBNNF NBNNSD
'ROTA                                                          '
     1     4     5                    $ IMPRE NIVEA1 NIVEA2
     0     0                          $ NBNNF NBNNSD
  0.18000E+03  0.00000E+00  0.00000E+00 $ TETA. X. Y.
'RECO'
     1     4     5     6  0.02000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS
     0     0                                              $ NBNNF NBNNSD
'RENC'
     1     6     7
'SAUV                                                          '
     1     7     0                    $ IMPRE NINOPO NTNOPO
 T2OUT.NOPO
 $ NOM FICHIER
'FIN                                                           '
```

Table 2: The definition of the outer 2D structure (`T2OUTNOPO.DATA`)

a lower circular electrode with dimensions smaller than the total lower surface of the quartz resonator. The choice of the number of distinct sub-domains results from the necessity of using different mesh procedures depending on the region we consider (triangular mesh for a region defined by an odd number of sides, rectangular mesh for a region defined by an even number of sides).

The definition of the various reference numbers of the different surfaces, and the translation from the references numbers defined in the 2D structures to the reference numbers in the 3D structures, is realized by the module `ma23xx` which is described in great details in the Modulef manual page 3-14, node 57 [1].

Since we already rotated and pasted the pieces together in the previous `apnoxx` step, this `apn3xx` step is mainly focused with re-numbering the elements and the sub-domains, and pasting the final two pairs of 3D pieces together in order to define the QCM with a finite counter electrode (while the sensing surface is fully coated with the grounded electrode).

The counter electrode is defined by reference number 4, the sensing electrode (covering the whole top surface of the QCM) as reference 3, and the other (non-coated) parts of the crystal are referred to by number 2 (reference number 1 disappeared when the two sub-elements were glued together).

[1] we will refer to parts of the Modulef manual by their web page reference: 3-14 here means Guide3-14/node57.html

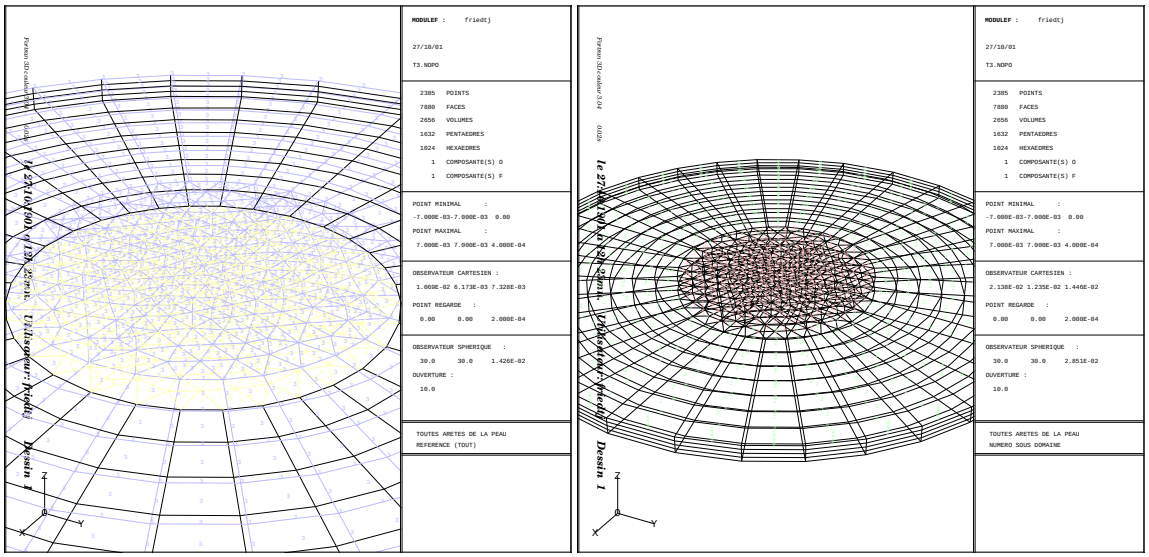

Figure 2: The final 3D structure after expanding the 2D structures developed in the previous part, and joining them together, with the display of the two distinct sub-domains (right).

```
'SUITE EXEMPLE 3D                                                    '
'INTR                                                                '
     1     0                          $ IMPRE NINOPO ( SD EXTERIEURE )
 T2IN.NOPO
'INTR                                                                '
     1     1                          $ IMPRE NINOPO ( SD EXTERIEURE )
 T2OUT.NOPO
$ NOM DU FICHIER STRUC IN DOWN
'MA23                                                                '
     1     0     7                    $ IMPRE NIVO2D NIVO3D
$ ===  DEFINITION DE LA FONCTION  ===
 TRAN
     6                                          $ SECTION SUPERIEUR
  0.0000000E+00  0.0000000E+00  0.0500000E-03    $ VECTEUR TRANSLATION
 BASE      -0.0000000E+00                       $ LA BASE
 FIN
 $ FIN DE LA DEFINITION DE LA FONCTION
 $ ===========  LES OPTIONS  =========
 REF
 FAIN  4  0  0  0
 SDSD  0  6  1  1      $ numero de sous domaine
 SDSD  0  6  2  2      $ numero de sous domaine
 F
 $ =======  APPEL DU MAILLEUR  =======
 GO
 $ STRUCT IN UP
'MA23                                                                '
     1     0     8                    $ IMPRE NIVO2D NIVO3D
$ ===  DEFINITION DE LA FONCTION  ===
 TRAN
     2                                          $ SECTION SUPERIEUR
  0.0000000E+00  0.0000000E+00  0.0500000E-03    $ VECTEUR TRANSLATION
 BASE       0.3000000E-03                       $ LA BASE
 FIN
 $ FIN DE LA DEFINITION DE LA FONCTION
 $ ===========  LES OPTIONS  =========
 REF
 FASU  3  0  0  0      $ reference face haut=electrode 3
 SDSD  0  2  1  1      $ numero de sous domaine
 SDSD  0  2  2  2      $ numero de sous domaine
 F
 $ =======  APPEL DU MAILLEUR  =======
 GO
$ STRUC OUT DOWN
'MA23                                                                '
     1     1     9                    $ IMPRE NIVO2D NIVO3D
$ ===  DEFINITION DE LA FONCTION  ===
 TRAN
     6                                          $ SECTION SUPERIEUR
  0.0000000E+00  0.0000000E+00  0.0500000E-03    $ VECTEUR TRANSLATION
 BASE      -0.0000000E+00                       $ LA BASE
 FIN
 $ FIN DE LA DEFINITION DE LA FONCTION
 $ ===========  LES OPTIONS  =========
 REF
 SDSD  0  6  1  1      $ numero de sous domaine
 SDSD  0  6  2  2      $ numero de sous domaine
 F
 $ =======  APPEL DU MAILLEUR  =======
 GO
$ STRUC OUT UP
'MA23                                                                '
     1     1     10                   $ IMPRE NIVO2D NIVO3D
$ ===  DEFINITION DE LA FONCTION  ===
 TRAN
     2                                          $ SECTION SUPERIEUR
  0.0000000E+00  0.0000000E+00  0.0500000E-03    $ VECTEUR TRANSLATION
 BASE       0.3000000E-03                       $ LA BASE
 FIN
 $ FIN DE LA DEFINITION DE LA FONCTION
 $ ===========  LES OPTIONS  =========
 REF
 FASU  3  0  0  0      $ reference face haut=electrode 3 ... FAIN  4  0  0  0
 SDSD  0  2  1  1      $ numero de sous domaine
 SDSD  0  2  2  2      $ numero de sous domaine
 F
 $ =======  APPEL DU MAILLEUR  =======
 GO
'RECO'
     1     7     8     2  0.01000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS IOPT
     0     0                                              $ NBNNF NBNNSD
'RECO                                                                '
     1     9    10     3  0.01000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS IOPT
     0     0                                              $ NBNNF NBNNSD
'RECO                                                                '
     1     2     3     5  0.01000E-03     0       $ IMP NIV1 NIV2 NIV3 EPS IOPT
     0     0                                              $ NBNNF NBNNSD
'RENE'
     1     5     6
'SAUV'
 T3.NOPO
'FIN'
```

Table 3: The definition of the 3D structure (`T3NOPO.DATA`)

2 Defining the interpolations using `comaxx`

The `comaxx` processor is used for assigning the required finite element to a given sub-domain. As mentioned earlier, our fundamental domains are distinguished by the number of side they are defined by in 2D (odd or even number of sides leading to triangular or rectangular finite elements). The piezoelectric finite element `PENT PR1D` is assigned to sub-domain 1 (odd number of sides) and `HEXA PQ1D` is assigned to sub-domain 2 (even number of sides). The resulting data arrays are stored in the output files `mail` and `coor` (these names are arbitrarily chosen by the user).

```
    0                                $ Y A T IL DES FONCTIONS INTERPRETEES
    3    2    0                      $ NDIM   NDSD   NBSDC
    4    0                           $ NNR    NBLC
    4    0
ELAS                                 $ NOM DE LA BIBLIOTHEQUE
    1                                $ NTYED DU SD      1
PENT PR1D                            $ LE NOM DES ELEMENTS DROITS
    0                                $ NTYEC DU SD      1
    1                                $ NTYED DU SD      2
```

```
HEXA PQ1D                            $ LE NOM DES ELEMENTS DROITS
    0                                $ NTYEC DU SD      2
T3.NOPO                              $ NOM DU FICHIER
    0                                $     ET NIVEAU DE LA SD NOPO
mail                                 $ NOM DU FICHIER
    0                                $     ET NIVEAU DE LA SD MAIL
coor                                 $ NOM DU FICHIER
    0                                $     ET NIVEAU DE LA SD COOR
    0    0                           $ NTMAIL  NTCOOR
```

Table 4: The definition of the interpolation methods (`T.COMAD`)

3 Material definition using `fomixx`

Definition of the physical properties of the material and the physical conditions under which the experiment is performed (external forces/heat sources) is done by `fomixx`. This program helps defining the two arrays required for defining the physical parameters of our problem: `FORC` for the external forces, and `MILLI` for the material properties.

```
'                                                                '
 forc                                $ NOM DU FICHIER DE LA S.D FORC
    1    1                           $ SON NIVEAU ET NB DE SES TAB. ASSOCIES
 mili                                $ NOM DU FICHIER DE LA S.D MILI
    1    1                           $ SON NIVEAU ET NB DE SES TAB. ASSOCIES
 $  DONNEES RELATIVES A LA S.D. FORC  $
  for       5     24                  $ NOM TYPE NBREMOT
        .000000000D+00                 $ for (  1)
        .000000000D+00                 $ for (  2)
        .000000000D+00                 $ for (  3)
        .000000000D+00                 $ for (  4)
        .000000000D+00                 $ for (  5)
        .000000000D+00                 $ for (  6)
        .000000000D+00                 $ for (  7)
        .000000000D+00                 $ for (  8)
        .000000000D+00                 $ for (  9)
        .000000000D+00                 $ for ( 10)
        .000000000D+00                 $ for ( 11)
        .000000000D+00                 $ for ( 12)
  ' force surfaciques nulles sur ref 2                          '  $ CONTENU
    1                                  $ NDSM
    2    0    0    0    0    0        0    0
    1    0    2    1                  $ NOSD NFRO NOPT ITRAIT (nopt=2=>notel)
for     1                              $ NTABL IADR
    2    0    2    1                  $ NOSD NFRO NOPT ITRAIT (nopt=2=>notel)
for     1                              $ NTABL IADR
 $  DONNEES RELATIVES A LA S.D. MILI  $
  mil       5     90                  $ NOM TYPE NBREMOT
       .867400000D+05                  $ mil (C11)
      -.065824831D+05                  $ mil (C12)
       .254824831D+05                  $ mil (C13)
       .083533936D+05                  $ mil (C14)
       .000000000D+00                  $ mil (C15)
       .000000000D+00                  $ mil (C16)
       .125255122D+06                  $ mil (C22)
       .039350995D+05                  $ mil (C23)
      -.100134939D+05                  $ mil (C24)
       .000000000D+00                  $ mil (C25)
       .000000000D+00                  $ mil (C26)
       .846346784D+05                  $ mil (C33)
```

```
       .136073615D+05                  $ mil (C34)
       .000000000D+00                  $ mil (C35)
       .000000000D+00                  $ mil (C36)
       .499650995D+05                  $ mil (C44)
       .000000000D+00                  $ mil (C45)
       .000000000D+00                  $ mil (C46)
       .627244245D+05                  $ mil (C55)
       .145412087D+05                  $ mil (C56)
       .350905754D+05                  $ mil (C66)
       .171000000D+03                  $ mil (e11)
      -.094902059D+03                  $ mil (e12)
      -.076097940D+03                  $ mil (e13)
       .094181799D+03                  $ mil (e14)
       .000000000D+00                  $ mil (e15)
       .000000000D+00                  $ mil (e16)
       .000000000D+00                  $ mil (e21)
       .000000000D+00                  $ mil (e22)
       .000000000D+00                  $ mil (e23)
       .000000000D+00                  $ mil (e24)
       .093952698D+03                  $ mil (e25)
      -.037566503D+03                  $ mil (e26)
       .000000000D+00                  $ mil (e31)
       .000000000D+00                  $ mil (e32)
       .000000000D+00                  $ mil (e33)
       .000000000D+00                  $ mil (e34)
      -.133433496D+03                  $ mil (e35)
       .053352698D+03                  $ mil (e36)
      -.392000000D+02                  $ mil (eps11)
       .000000000D+00                  $ mil (eps12)
       .000000000D+00                  $ mil (eps13)
      -.404033857D+02                  $ mil (eps22)
      -.008473235D+00                  $ mil (eps23)
      -.397966142D+02                  $ mil (eps33)
  ' mat Quartz AT                                               '  $ CONTENU
    2    0    0    0    0    0    0    0
    1    0    2    1                  $ NOSD NFRO NOPT ITRAIT (nopt=notel=2)
mil     1                              $ NTABL IADR
    2    0    2    1                  $ NOSD NFRO NOPT ITRAIT (nopt=notel=2)
mil     1                              $ NTABL IADR
```

Table 5: The definition of the material properties and external forces (`T.FOMID`)

The numerical values of the piezoelectric material for an AT-cut quartz crystal is obtained using the Matlab script and the numerical values given in table 6.

The numerical values of the piezoelectric material for an AT-cut quartz

4 Assembling the data structures `thelxx`

The various data structures created in the previous steps are assembled using `thelxx`. As mentioned in the manual (Guide7-14/node174.html), the `poba` temporary data file is required and must be defined in the script used to run `thelxx`

```
function [M,Kp]=simul(a,K)

%function SIMUL for trnasfer of rigidity matrix K
%in rotated coordinates by matrix a
%OUT : results are given in Kp (= K')

C = K(1:6,1:6)
e = K(7:9,1:6)
v = K(7:9,7:9)

%Upper Left part of M
M(1:3,1:3) = a.^2

%Upper right part of M
M(1,4) = 2*a(1,2)*a(1,3)
M(1,5) = 2*a(1,3)*a(1,1)
M(1,6) = 2*a(1,1)*a(1,2)
M(2,4) = 2*a(2,2)*a(2,3)
M(2,5) = 2*a(2,3)*a(2,1)
M(2,6) = 2*a(2,1)*a(2,2)
M(3,4) = 2*a(3,2)*a(3,3)
M(3,5) = 2*a(3,3)*a(3,1)
M(3,6) = 2*a(3,1)*a(3,2)

%Lower Left part of M
M(4,1) = a(2,1)*a(3,1)
M(4,2) = a(2,2)*a(3,2)
M(4,3) = a(2,3)*a(3,3)
M(5,1) = a(3,1)*a(1,1)
M(5,2) = a(3,2)*a(1,2)
M(5,3) = a(3,3)*a(1,3)
M(6,1) = a(1,1)*a(2,1)
M(6,2) = a(1,2)*a(2,2)
M(6,3) = a(1,3)*a(2,3)

%Lower Right part of M

M(4,4) = a(2,2)*a(3,3)+a(2,3)*a(3,2)
M(4,5) = a(2,1)*a(1,1)+a(2,3)*a(3,1)
M(4,6) = a(2,2)*a(3,1)+a(2,1)*a(3,2)
M(5,4) = a(1,2)*a(3,3)+a(1,3)*a(3,2)
M(5,5) = a(1,3)*a(3,1)+a(1,1)*a(3,3)
M(5,6) = a(1,1)*a(3,2)+a(1,2)*a(3,1)
M(6,4) = a(1,2)*a(2,3)+a(1,3)*a(2,2)
M(6,5) = a(1,3)*a(2,1)+a(1,1)*a(2,3)
M(6,6) = a(1,1)*a(2,2)+a(1,2)*a(2,1)

%Calcul de la transformee
disp('Transformee')

Cp = M*C*M'
ep = a*e*M'
vp = a*v*a'

Kp = [Cp ep';ep vp]
disp('Fini, bon amusement !')

format long
```

```
  8.6740000e+10   6.9900000e+09   1.1910000e+10  -1.7910000e+10   0.0000000e+00   0.0000000e+00   1.7100000e-01   0.0000000e+00   0.0000000e+00
  6.9900000e+09   8.6740000e+10   1.1910000e+10   1.7910000e+10   0.0000000e+00   0.0000000e+00  -1.7100000e-01   0.0000000e+00   0.0000000e+00
  1.1910000e+10   1.1910000e+10   1.0720000e+11   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00
 -1.7910000e+10   1.7910000e+10   0.0000000e+00   5.7940000e+10   0.0000000e+00   0.0000000e+00  -4.0600000e-02   0.0000000e+00   0.0000000e+00
  0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   5.7940000e+10  -1.7910000e+10   0.0000000e+00   4.0600000e-02   0.0000000e+00
  0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00  -1.7910000e+10   3.9875000e+10   0.0000000e+00  -1.7100000e-01   0.0000000e+00
  1.7100000e-01  -1.7100000e-01   0.0000000e+00  -4.0600000e-02   0.0000000e+00   0.0000000e+00   3.9200000e-11   0.0000000e+00   0.0000000e+00
  0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   4.0600000e-02  -1.7100000e-01   0.0000000e+00   3.9200000e-11   0.0000000e+00
  0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   0.0000000e+00   4.1000000e-11
```

Table 6: Matlab script for rotating by the appropriate angle ($90 - 35.15^o$ around the X axis) the parameters defining the piezoelectric properties of quartz, and matrix defining the piezoelectric properties of quartz used when executing this script.

```
mail                                $ NOM DU FICHIER
    1                               $     ET NIVEAU DE LA SD MAIL
coor                                $ NOM DU FICHIER
    1                               $     ET NIVEAU DE LA SD COOR
tae                                 $ NOM DU FICHIER
    1                               $     ET NIVEAU DE LA SD TAE
    0                               $ NTTAE
    1                               $ 1 SI POBA EST UTILISEE , 0 SINON
/imec/users/friedtj/modulef99/linux/sta/etc/poba.direct
                                    $ NOM DU FICHIER POBA
    1                               $ 1 SI MILI EST UTILISEE , 0 SINON
```

```
mili                                $ NOM DU FICHIER
    1                               $     ET NIVEAU DE LA SD MILI
    1                               $ 1 SI FORC EST UTILISEE , 0 SINON
forc                                $ NOM DU FICHIER
    1                               $     ET NIVEAU DE LA SD FORC
    2                               $ NPROV
    0                               $ NTHELA
    0    1    1    1                $ IOPT(*)
:RIE    0                           $ NOM DU TABLEAU DES CL ET NOMBRE DE CL
VIDE       1                        $ NOMCOU LVECT
```

Table 7: The definition of the data structures assembling methods (`DATA.THELD`)

5 Defining boundary parameters: `cobdxx`

The boundary conditions on each of the various surfaces defined by their respective reference numbers are defined using `cobdxx`.

In our case, we define two sets of boundary conditions leading to 5 explicit boundary conditions:
- we forbid any displacement of the sensing electrode (reference 3) by requiring that the 3 degrees of freedom (1, 2, 3) of the displacement variable (`VN`) are kept at 0
- we apply voltages to the electrodes: the sensing electrode (reference 3) is kept at ground level and the counter electrode is polarized at 0.5 V. These conditions are set by defining the electric potential degree of freedom (`PHIE`) to 0.0 value for faces referenced by number 3, and a value of 0.5E-3 kV for faces referenced by number 4 (counter electrode).

The unit (kV for the electric potential) is chosen in order to be coherent with the other units used in defining the material properties, leading to a matrix filled with number closer to 1 than they would if S.I. units had been chosen (cf manual Guide7-17/node174.html).

```
mail                                    $ NOM DU FICHIER
   35                                   $     ET NIVEAU DE LA SD MAIL
bdcl                                    $ NOM DU FICHIER
   35                                   $     ET NIVEAU DE LA SD BDCL
    0                                   $ NTBDCL
    1    5    5                         $ ICONST  NBFR  NTYP
    3    1  VN                          $ REF   INC.VARIATIONNELLE  MNEMO
    3    2  VN                          $ REF   INC.VARIATIONNELLE  MNEMO
    3    3  VN                          $ REF   INC.VARIATIONNELLE  MNEMO
```

```
    3    4  PHIE                       $ REF   INC.VARIATIONNELLE  MNEMO
    4    4  PHIE                       $ REF   INC.VARIATIONNELLE  MNEMO
0.0000000E+00                           $ VAL: pas bouger dans les 3D sur la ...
0.0000000E+00                           $ VAL  ... face 1
0.0000000E+00                           $ VALEUR idem ...
0.0000000E+00                           $ VALEUR potentiel electrode 3
0.5000000E-03                           $ VALEUR potentiel electrode 4 (kV)
   0                                    $ 1 SI SD NDL1
   0                                    $ 2 SI CL EN RL A LA MAIN ; -1 SI CL EN RL PAR SP
```

Table 8: The definition of the boundary conditions (`DATA_LIM.COBDD`)

6 Solving the problem: `crouxx`

Once all the data arrays are defined (geometrical definition of the object, interpolation using the right finite elements, material properties, boundary conditions), the problem can be solved using `crouxx`.

```
mail                                    $ NOM DU FICHIER
   33                                   $     ET NIVEAU DE LA SD
    1    5    4                         $ NDSM  NTYP  ND
tae                                     $ NOM DU FICHIER
   22                                   $     ET NIVEAU DE LA SD
    1                                   $ 1 SI BDCL EST UTILISE , 0 SINON
```

```
bdcl                                    $ NOM DU FICHIER
   15                                   $     ET NIVEAU DE LA SD BDCL
    0                                   $ 1 SI CL. EN RL. EXISTE
sol.b                                   $ NOM DU FICHIER
    4                                   $     ET NIVEAU DE LA SD
    1                                   $ IMPREB
```

Table 9: The script for solving the problem `DATA.CROUD`)

7 Displaying the result: `trc3xx`

The results of the calculation are displaced using the `trc3xx` processor. The potential `PHIE` is displayed in figure 3 (left) while the displacement fields are displayed in figures 3 (right) and 4. The combination of the fields of the displacements in the three directions leads to a vector display as depicted in figure 5.

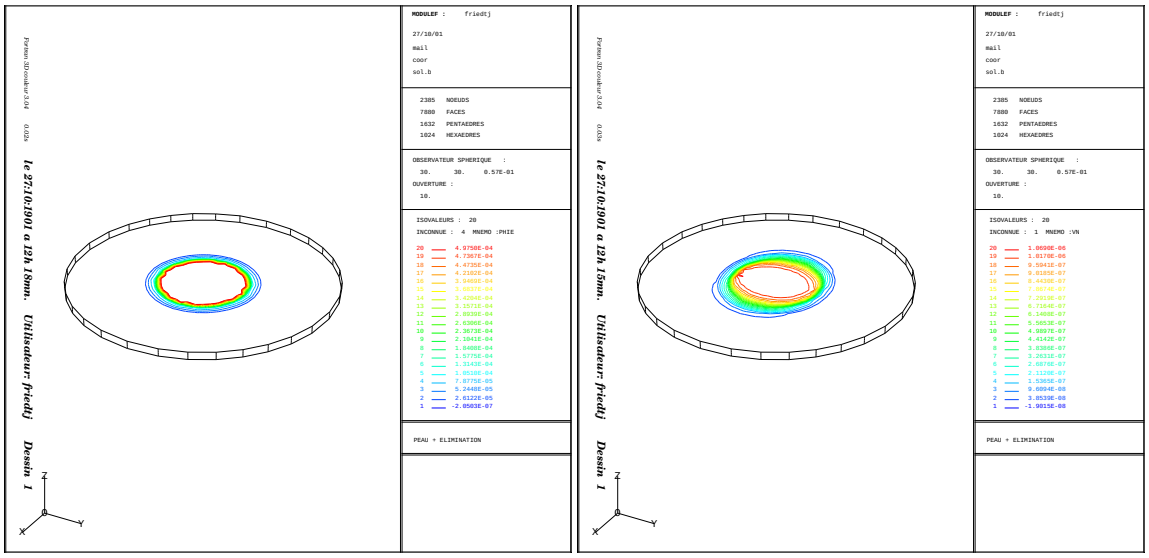

Figure 3: Display of the potential (voltage) distribution and the amplitude of the displacement in the main displacement axis (X).

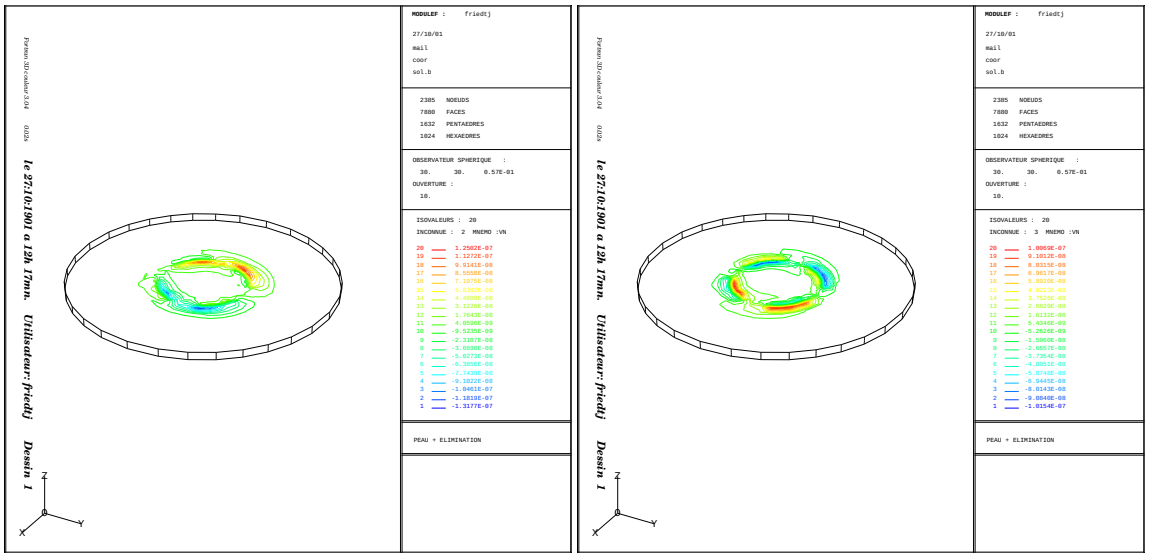

Figure 4: Display of the amplitude of the displacement in the two other displacement axis (Y and Z).

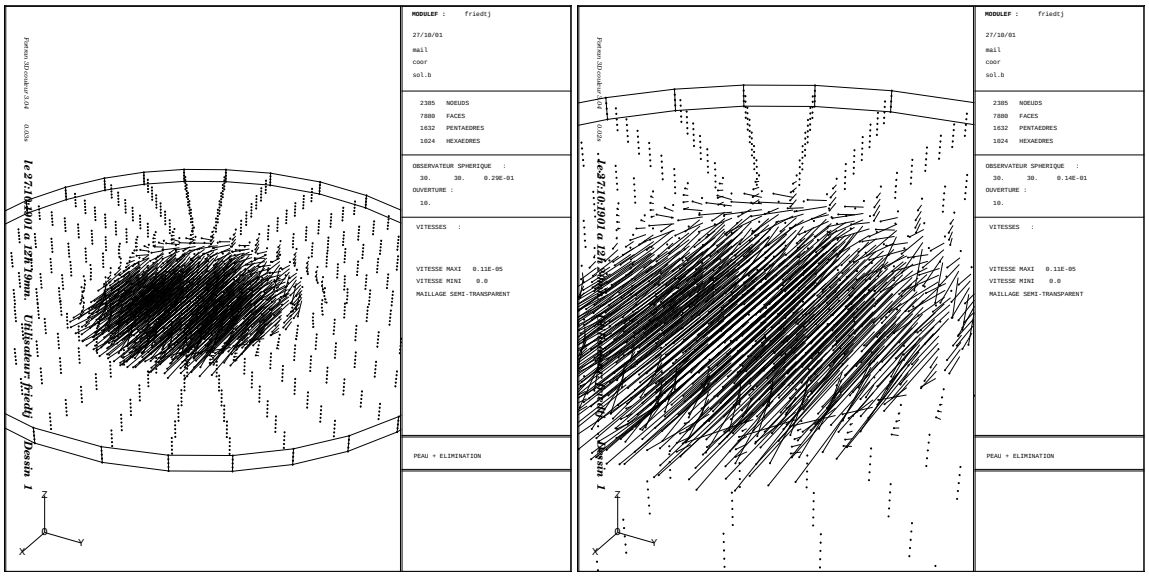

Figure 5: Display of the velocity field, combining the informations of the 3 displacement matrices .

8 Conclusion

Finite element analysis leads to complementary results on the displacement of the QCM to the analytical analysis. The magnitude of the displacement is in agreement with the analytical solution [1, 2] with an amplitude in the pm range when a DC potential of 0.5 V is applied. Considering our QCMs, when oscillating in liquid, display a quality factor $Q \simeq 1000 - 3000$, we conclude that the amplitude of the oscillations are in the nm range.

We also believe we can consider the relative displacement in the X direction and the Z direction to be correctly predicted by finite element analysis, and calibrate the displacement in the X direction from analytical resolution of the problem.

In this particular case, finite element analysis allows us to estimate the displacement in the

Z direction, which cannot be predicted by analytical resolution since it is a side effect of the finite extension of the counter electrode. The analytical resolution of the problem of knowing the displacement of a piezoelectric substrate of infinite dimensions in the (X, Y) plane, to which a DC potential is applied, predicts a displacement only in the X direction, which can be verified by finite element analysis (the main displacement component is also in that direction).

In our case, the displacement of the QCM surface in the Z direction is of major importance as it leads to longitudinal waves in the liquid above the QCM surface, which is the source of frequency fluctuations as the resonator is disturbed by the standing wave. We conclude from finite element analysis that this component is about 1/10th of the X displacement and is thus not negligible in understanding the origin of longitudinal waves in the liquid which disturb the oscillation of the resonator and thus its frequency stability.

```
all:sol.b

T2IN.NOPO: T2INNOPO.DATA
echo "E T2INNOPO.DATA F" | apnoxx xargs

T2OUT.NOPO: T2OUTNOPO.DATA
echo "E T2OUTNOPO.DATA F" | apnoxx xargs

T3.NOPO: T3NOPO.DATA T2IN.NOPO T2OUT.NOPO
echo "E T3NOPO.DATA F" | apn3xx xargs

coor: T.COMAD T3.NOPO
echo "E T.COMAD 5 F" | comaxx xargs

forc: T.FOMID coor
echo "E TRHO.FOMID 5 F" | fomixx xargs

# echo "E T.FOMID 5 F" | fomixx xargs
# echo "E TFORC.FOMID 5 F" | fomixx xargs

tae: DATA.THELD forc
echo "E DATA.THELD 5 F" | thelxx xargs

bdcl: DATA_LIM.COBDD tae
echo "E DATA_LIM.COBDD 5 F" | cobdxx xargs
# echo "E DATA_TMP.COBDD 5 F" | cobdxx xargs
# echo "E DATA.COBDD 5 F" | cobdxx xargs

sol.b: DATA.CROUD bdcl
echo "E DATA.CROUD 5 F" | ./crouxx xargs

clean:
\rm T2IN.NOPO T2OUT.NOPO T3.NOPO coor forc mili tae mail bdcl sol.b core
```

Table 10: The `Makefile` for automatically running the whole simulation.

References

[1] Bret A. Martin and Harold E. Hager. Velocity profile on quartz crystals oscillating in liquids. *J. Appl. Phys.*, 65(7):2630–2635, 1989. 7

[2] K. Keiji Kanazawa. Mechanical behaviour of films on the quartz microbalance. *Faraday Discuss.*, 107:77–90, 1997. 7