Development of Microsystems Analysis (µsys) Software Using Hybrid Finite Elements and Direct Solution of Coupled Equations

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Abstract

In this work, we describe the development and implementation of a hybrid finite element based software "µsys" for the analysis of coupled multi-physical phenomena encountered in Micro-Electro-Mechanical Systems (MEMS) or microsystems. The developed computational strategy entails the use of hybrid finite elements for modeling structures, which overcomes some of the inherent shortcomings associated with the interpolation incompatibility of the finite elements. As a result, a coarse mesh with a single type of high aspect ratio element can be used for computationally efficient solution of many kinds of coupled partial differential equations. The same element is used to interpolate multiple state variables including displacement, temperature, fluid pressure and electric potential etc. Additionally, we use direct, rather than staggered, approach to solve coupled PDEs. The µsys software has modular architecture to seamlessly interface the analysis codes with various packages having pre and post-processing capabilities. This helps the user to work with familiar and accessible pre- and post-processing environments while using µsys as the versatile finite element analysis engine. We illustrate the architecture and working of µsys with two coupled analysis modules, viz., coupled structure-electrostatics and coupled structure-squeeze film. Pre- and post-processing capabilities of a commercial finite element software are used to demonstrate working with µsys as an example.

Keywords: Coupled PDEs, MEMS, Multi-physics, Squeeze-film, Pull-in

Introduction.

Micro-Electro-Mechanical Systems (MEMS) or microsystems are ubiquitous in many consumer products and industrial applications today. Simulation and design of microsystem components and devices is indispensable to achieve improved performance and cost-effective manufacturing. Various computational platforms are available to perform numerical modeling and finite element analysis of multi-physical phenomena associated with the microsystems [1-4]. Solving coupled partial differential equations in continuous domain and ordinary differential equations in the reduced order models is unique to microsystems.

The earliest published work [5] advocated the strategy of staggered coupling of PDE solvers and focused on 'wrappers' that exchanged data between different modules during simulation. For example, in MEMCAD (which is now known as Coventorware), commercial finite element software ABAQUS was used for elastic analysis and in-house developed FASTCAP was used for electrostatic analysis. MEMCAD's wrapping code called ABAQUS and FASTCAP alternately to find self-consistent solution of PDEs of elastic and electrostatic domains. The main focus of MEMCAD then was on emulating microfabrication process and building CAD models as well as post-processing. A comprehensive review of developments related to process modeling and visulaization tools for MEMS can be found in [6]. The staggered approach of alternating between solvers of different physical domains is prevalent even now.

In μsys we take a different approach. We have a single integrated analysis engine that can be interfaced with any pre- and post-processing modules of other software. This is motivated by two commonly encountered problems in existing microsystems simulator software. First, the user should be familiar with types of finite elements to be used for meshing the CAD model. It is very common to have many types of elements to be used for meshing the CAD model also it is common to have different element types, one for each type of coupled simulation, in the existing softwares. The users should also be aware of the dangers of coarse meshing, distortion in the elements in the mesh and aspect ratio of the elements (which should ideally be close to unity) to avoid converged but inaccurate results. Interdisciplinary users of microsystem cannot be expected to have intimate knowledge of finite elements and PDEs of many physical domains. Second, the staggered approach is computationally inefficient and leads to prolonged simulation time.

The two shortcomings of existing microsystems software are overcome in μsys by using hybrid finite elements. In hybrid finite elements, displacement and stress (i.e; the state variable and its derivative) are independently interpolated to avoid the incompatibility in the interpolation functions and ensuing problem of "locking" phenomena [7,8]. In a hybrid finite element, aspect ratio need not be close to unity and the element need not be very small to give accurate results. A single 3D element type can cater to solve multiple PDEs. Only one element across the thickness of a MEMS component is enough and this element can be very large in the in-plane dimensions. This makes it possible to get accurate results with coarse meshes [9-11]. The single 3D hybrid finite element type can be endowed with multiple state variables, namely, displacement, pressure, temperature, electric potential etc. This enables simultaneous solution of multiple coupled PDEs directly [12-15] rather than in the staggered manner of most existing software today. Based on the foregoing, the focus in μsys is on a single analysis engine that is developed in-house. This analysis engine is easily linked with any pre- and post-processors.

In the next section, we discuss overall architecture of μsys. Analysis module of μsys is discussed later by illustrating briefly implementation and working of two analysis sub-modules, coupled structure-electrostatics and coupled squeeze film, respectively. The use of pre- and post-processing capabilities of finite element software NISA [16], are demonstrated by use of appropriate data parsing.

Architecture of μsys

The overall system architecture of μsys is shown in Figure 1. As is common with simulation softwares, μsys is divided into three modules namely, pre-processing, analysis and post-processing. Our focus is only in the development of μsys on finite element analysis module by, relying on commercially available platforms for pre and post-processing through appropriate data parsing. Preprocessors are used to create CAD models, finite element meshing, specification of material data, loading data, boundary and initial conditions, etc. Pre-processing can be done using popular commercially available platforms such as NISA, ABAQUS, ANSYS etc. The task of developing an independent pre-processor is very involved, and also, as the users are generally accustomed to using at least one of the available pre-processing platforms. The input data to the analysis module of µsys can be generated by parsing appropriate information from the input file generated using pre-processor. Thus, the user models using accessible pre-processor, and parsers take care of input data format required for µsys. Any additional analysis dependent data specification can be done using data input section of µsys.

After the analysis, the output file generated by µsys, which consists of field variables such as stress, potential, displacement, etc., sought at different nodes, is parsed into appropriate post-processing format. Again, the commercially available post-processing tools can be used for visualization and graph plotting. The visualization of output using post-processing section of µsys is also another alternative. This development is partially completed.

As mentioned earlier, the primary focus of µsys development is on the finite element analysis section. Currently, structural, electrostatics and coupled analysis modules (see, Figure 1) are part of the µsys. The characteristic features and working with the two coupled modules, is the subject of discussion of the next section. In doing so, we have selected NISA [16] as a pre and post-processing platform of µsys as an example.

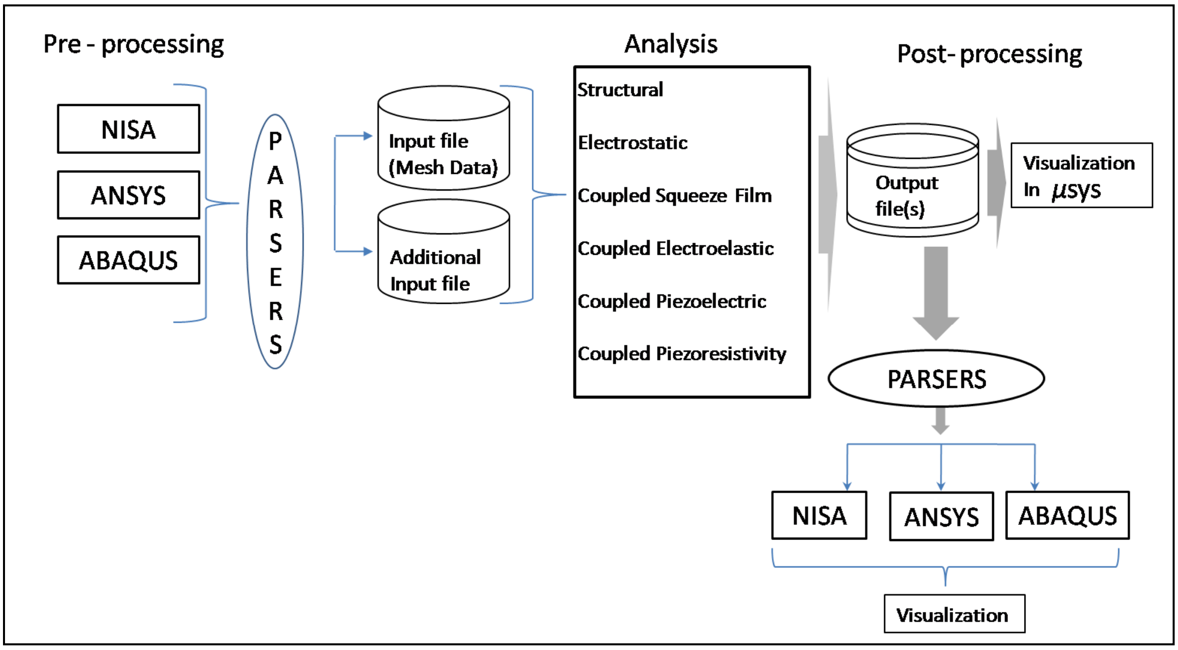

Figure 1: Architecture of µsys

Currently, six different analysis modules are implemented in µsys. It includes:

1. Structural
2. Electrostatics
3. Coupled structure-electrostatics or electroelastics

4. Coupled squeeze film
5. Coupled piezoelectric
6. Coupled piezoresistivity

In this section, we discuss coupled structure-electrostatics and coupled squeeze film modules as illustrative examples to demonstrate solver capabilities of μsys. Rest of the coupled modules are extension of the coupled structure-electrostatics with addition of analysis dependent data specification [12, 13].

Coupled structure-electrostatics module

Coupled structure-electrostatics is a very important module in the analysis of microsystems structures. The knowledge of static and dynamic pull-in voltages, capacitance, etc. is important for the design of electrostatic actuators and sensors.

In this section we briefly describe the finite element formulation of the elastic-electrostatic coupled problem. Detailed implementation of nonlinear structural hybrid finite element development can be found in [7] and [8]. For coupling with electrostatics [9, 10] and [13] may be consulted.

Strong form of equations for the structural problem in the reference configuration Ω (total domain) is given as

$$\nabla.(FS)+\rho_0 b^0 = 0, \quad \text{on} \quad \Omega \quad (1)$$

$$E=\overline{E}(u):=\frac{1}{2}\left[(\nabla u)+(\nabla u)^T\right], \text{ on } \Omega \quad (2)$$

$$S_{\text{mech}}=\tilde{S}(C), \quad \text{on} \quad \Omega \quad (3)$$

$$t^0 = FSn^0, \quad \text{on} \quad \Omega \quad (4)$$

$$t^0=\overline{t}^0, \quad \text{on} \quad \Gamma_t \quad (5)$$

$$u=0. \quad \text{on} \quad \Gamma_u \quad (6)$$

where $F(X):=\nabla\chi = I+\nabla u$, is the deformation gradient defined with respect to material coordinates X, u the displacement field, E the Lagrangian measure of strain, $C=F^T F$ the right Cauchy-Green strain tensor, S the second Piola-Kirchhoff stress, $t^0 =\| JF^{-T} n^0 \| t$ the tractions defined on the reference configuration in terms of tractions on the deformed configuration, $\rho_0 = J\rho$ the density in the reference configuration in terms of the density in the deformed configuration, $J=\det(F)$, n^0 the outward normal to Γ, S_{mech} is the constitutive equation of solid. The surface Γ, is the boundary between solid and surrounding consisting of open disjoint union of regions, $\Gamma=\overline{\Gamma_u\cup\Gamma_t}$ for structural problem.

For electrostatics, the governing equations are given by

$$\nabla . d = 0, \qquad \text{on} \quad \Omega \tag{7}$$

$$d = \sigma J C^{-1} e, \qquad \text{on} \quad \Omega \tag{8}$$

$$e = -\nabla_X \phi, \qquad \text{on} \quad \Omega \tag{9}$$

$$\phi = \overline{\phi}, \qquad \text{on} \quad \Gamma_\phi \tag{10}$$

$$d_n^0 = \overline{d_n^0}, \qquad \text{on} \quad \Gamma_d \tag{11}$$

$$S_{\mathrm{M}} = \varepsilon J \left[C^{-1}(e \otimes e) C^{-1} - \frac{(e.C^{-1}e)}{2} C^{-1} \right]. \tag{12}$$

where S_{M} is the Maxwell stress, e and d the Lagrangian electric field and electric displacement vectors, respectively, ϕ the electric potential or voltage, $d_n{}^0$ the normal electric displacement vector defined on the reference configuration, σ and ε are the conductivity and permittivity, respectively. The surface Γ, is the boundary between solid and surrounding consisting of open disjoint union of regions, $\Gamma = \overline{\Gamma_d \cup \Gamma_\phi}$ for electrostatic problem.

By enforcing Eqns. (1) and (7) in a weak sense, we get

$$\int_\Omega S : \overline{E_\delta}\, d\Omega = \int_\Omega \rho_0 u_\delta .\, b^0 d\Omega + \int_{\Gamma_t} u_\delta .\, \bar{t}^0 d\Gamma, \tag{13}$$

$$\int_\Omega \nabla\phi_\delta .\, (\sigma J C^{-1} \nabla\phi)\, d\Omega = -\int_{\Gamma_d} \phi_\delta \overline{d_n}\, d\Gamma \qquad \forall \phi_\delta, \tag{14}$$

where u_δ, E_δ and ϕ_δ denotes variation of displacement, strain and potential fields, respectively.

In a hybrid formulation, strain-displacement relation Eq. (2), is also enforced in a weak sense. Thus, we get

$$\int_\Omega (S)_\delta : \left[\overline{E}(u) - \widehat{E}(S) \right] d\Omega = 0, \tag{15}$$

where S_δ denotes the variation of stress field.

After linearization of Eqns. (13), (14) and (15) at the reference configuration, we get incremental formulations [9]. Introducing following interpolation

$$u = \mathrm{N}\hat{u}, \qquad \phi = \mathrm{N}\widehat{\phi}, \qquad S_{\mathrm{mech}} = \mathrm{P}\beta \tag{16}$$

and using the same shape functions N and P for increments, we get following finite element equations,

$$Q\hat{u}_\Delta + K_{u\phi}\hat{\phi}_\Delta + (G_0 + G^T)\beta_\Delta = (f_u)_{\Delta,} \tag{17}$$

$$K_{\phi S}\beta_\Delta + K_{\phi\phi}\hat{\phi}_\Delta = (f_\phi)_{\Delta,} \tag{18}$$

$$G\hat{u}_\Delta - H\beta_\Delta = (f_S)_\Delta . \tag{19}$$

Expressions for the matrices Q, G, H, $G_0, K_{u\phi}, K_{\phi\phi}, K_{\phi S}$ and the force vectors f_u, f_ϕ, f_S can be found in [9].

Example

The working of coupled elastic-electrostatics module is demonstrated using an example of static pull-in of a cantilever beam. Pre- and post-processing is done using the commercial FEM package NISA. Figure 2 shows the block-diagram of working with “NISA- µsys” system for coupled elastic-electrostatics problems.

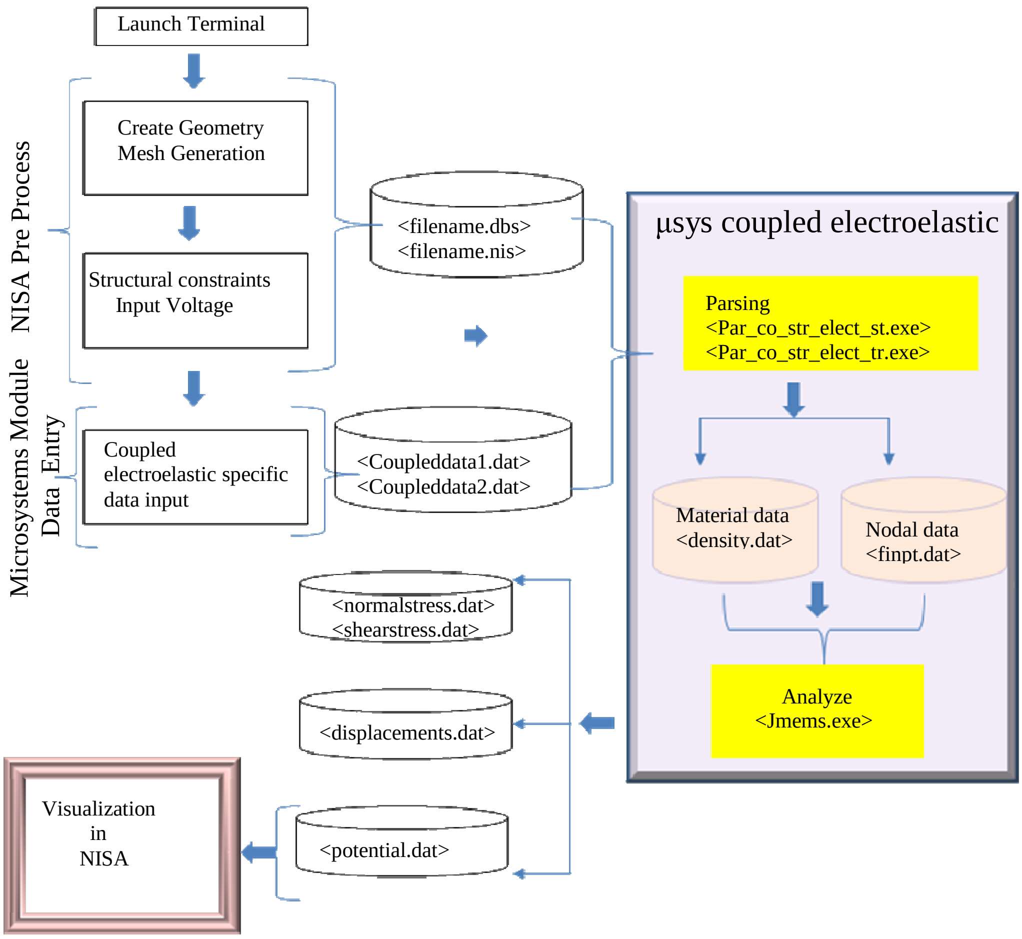

Figure 2: Block-diagram of NISA- µsys coupled elastic-electrostatics module

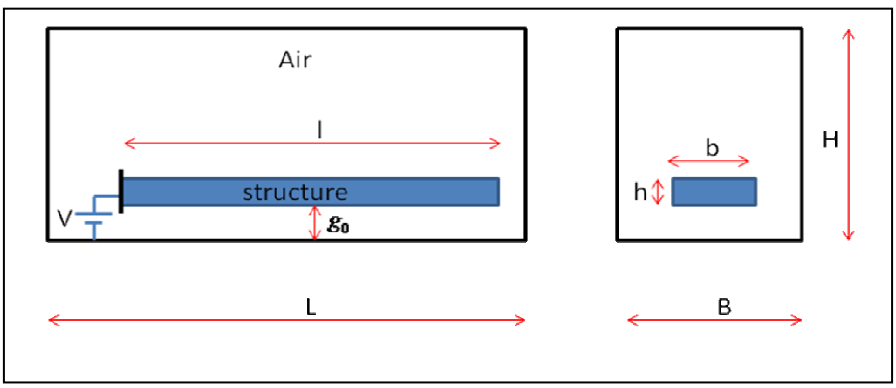

Figure 3: A Cantilever beam, ground, and the surrounding air domain

Figure 3 shows the schematic for a cantilever beam subjected to gradual increase in the voltage from 0 to static pull-in value. In the direct solution strategy, the air domain is modeled as a weak elastic dielectric material. The dimensions and properties for modeling elastic and air domains are given in Table 1.

Data	**Values**
Beam length (l)	100 μm
Beam width (b)	10 μm
Beam height (h)	0.5 μm
Surrounding domain box length (L)	140 μm
Surrounding domain box width (B)	60 μm
Surrounding domain box height (H)	52 μm
Initial gap (g)	1 μm
Young's modulus (beam)	169 GPa
Poisson's ratio (beam)	0.3
Density (beam)	2231 Kg/m^3
Relative permittivity (beam)	11.7
Electrical conductivity (beam)	1.56e-03 S/m
Young's modulus (air)	1.0e07 Pa
Poisson's ratio (air)	0.0
Density (air)	0.0 Kg/m^3
Relative permittivity (air)	1
Electrical conductivity (air)	5.5e-15 S/m

Table 1: Dimensions and material data for cantilever pull-in problem

Figure 4 shows the tip-deflection of cantilever beam as the voltage is increased from 0 till pull-in. Accurate calculation of deflection significantly affects determination of the pull-in voltage. Close to pull-in phenomena, the error in the deflection as computed by µsys and COMSOL is close to 16%. Table 2 gives comparison of the values for static pull-in obtained from µsys and COMSOL with analytical calculations. Figures 5 and 6 show the displacement and potential fields visualization in NISA. More comparative studies can be found in [13].

Method	**Static pull-in voltage (V)**
µsys	2.55
COMSOL	2.6
Analytical [19] Analytical [20]	2.53 2.55

Table 2: Static pull-in calculation for a cantilever beam

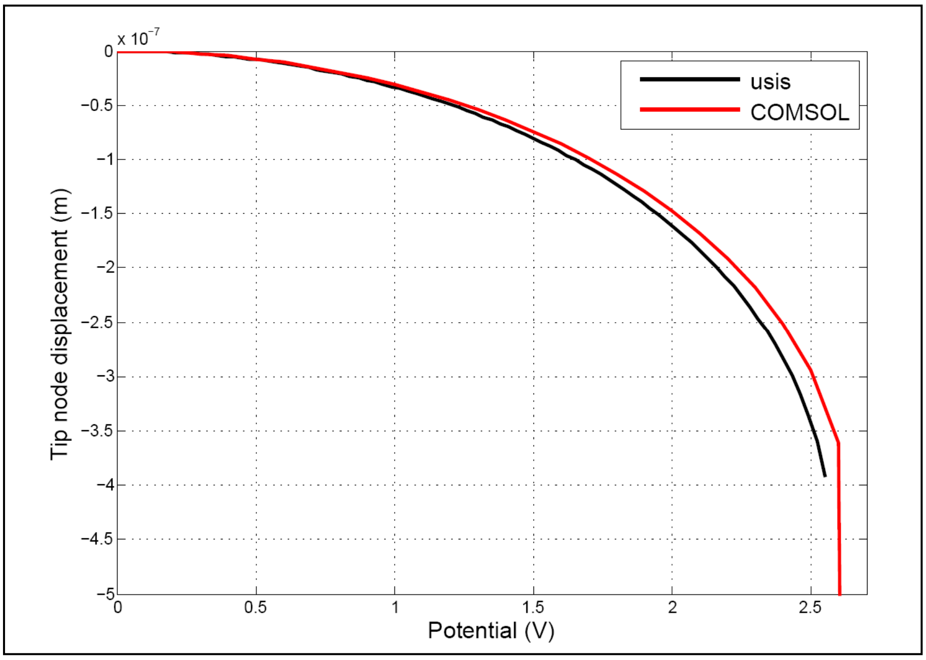

Figure 4: Tip deflection of a cantilever beam with increase in voltage

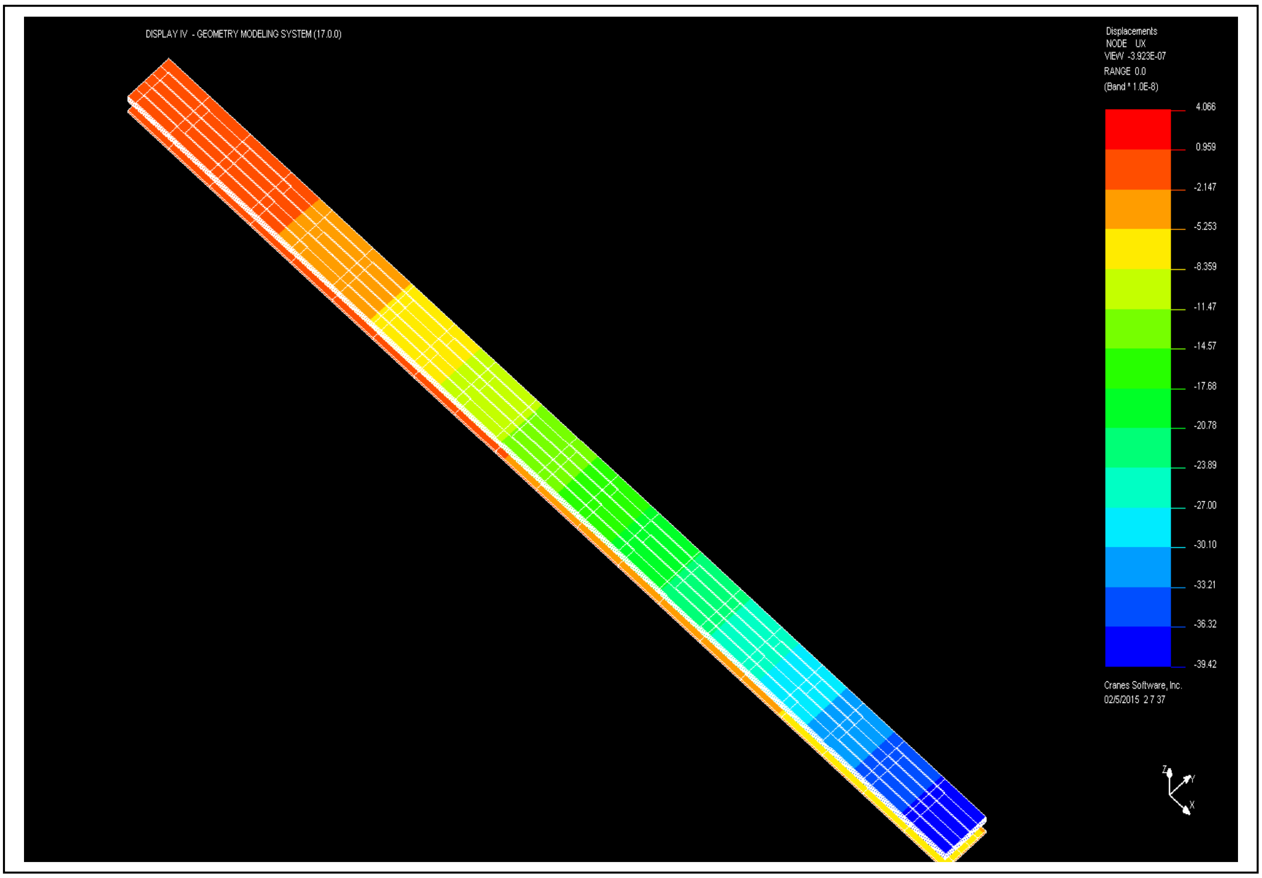

Figure 5: Displacement field visualization in NISA

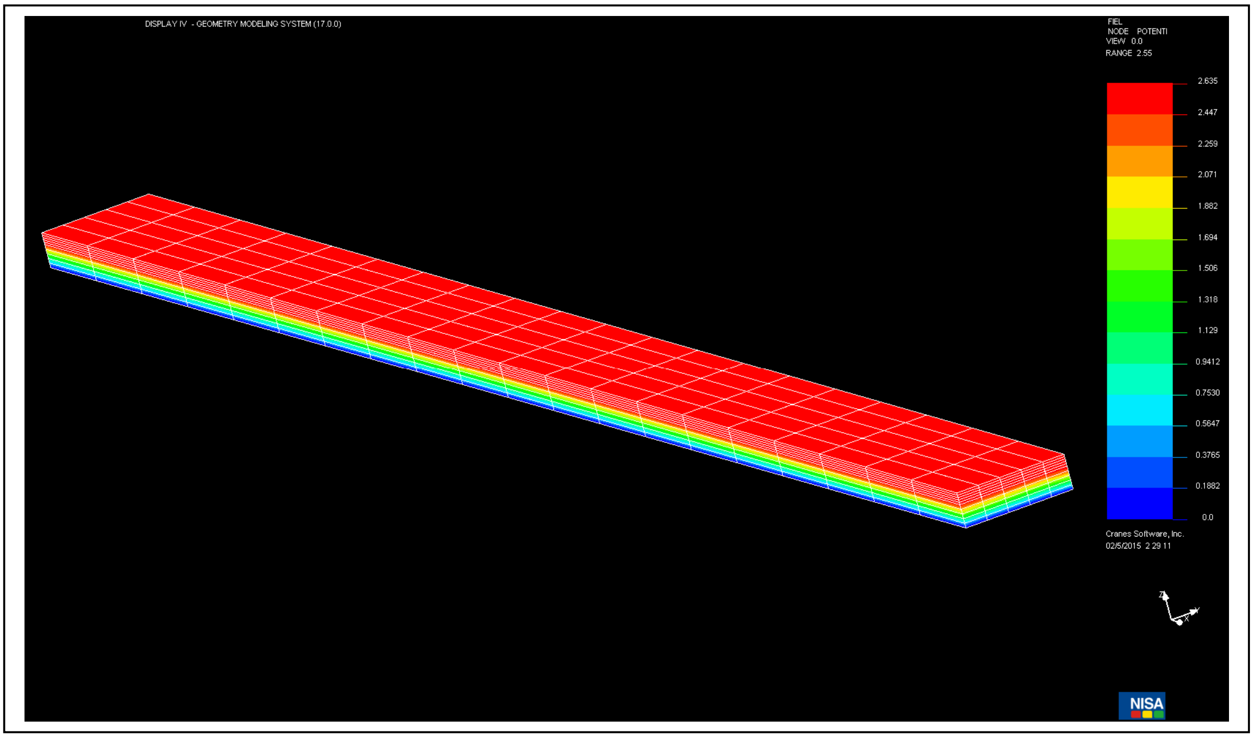

Figure 6: Potential field visualization in NISA

Coupled Squeeze-Film Analysis

The squeeze film effect is prevalent in vibratory MEMS devices where a thin film of air trapped between a fixed substrate and a plate vibrating normally to the fixed plate behaves like both a viscous damper and as an air spring [18]. Various attempts have been made to model the coupled fluid structure problem of squeeze film. A thorough review of the prior works can be found in [14] where we discussed a coupled finite element based methodology to solve the fluid-structure squeeze film problem. In the present software developed, we have implemented a coupled hybrid monolithic formulation. Hybrid elements are known to overcome locking issues faced with displacement based formulations in modeling high aspect ratio structures (as present in MEMS devices with squeeze film). Thus, our present formulation is able to show good results even for those mesh generators which are limited to lower order meshes and with far less number of elements compared to displacement based formulations.

In implementing the analysis module for squeeze film, we solve the 3D elasticity equation and the 2D Reynolds equation for squeeze film flow in a coupled method following the procedure outlined in [14]. For the dynamic structural problem without any body force, we have the following governing equation in a weighed integral sense for hybrid elements [15].

$$\int_{\Omega} u_{\delta} \cdot \left(\nabla . \tau - \rho \frac{\partial^2 u}{\partial t^2} \right) d\Omega + \int_{\Gamma} u_{\delta} \left(\bar{t} - t \right) d\Gamma + \int_{\Gamma} \tau_{\delta} : \left[\bar{\varepsilon}(u) - C^{-1} \tau \right] d\Omega = 0 \qquad (20)$$

where u is the displacement, τ the stress, t the traction, u_δ and τ_δ the variations in displacement and stress field respectively, C the constitutive matrix, $\bar{t}$ prescribed traction and $\bar{\varepsilon}(u) = (\nabla u) + (\nabla u)^T$. For coupled squeeze film problem with structural interaction, the wet surface (the surface in contact with air) is subject to the fluid pressure through traction $\bar{t} = -\tilde{p}\hat{n}$. We discretize Eqn. (20) using finite element interpolations for displacements and stress fields and their variations as, $u = N_u\hat{u}$, $u_\delta = N_u\hat{u}_\delta$, $\bar{\varepsilon}(u) = B_u\hat{u}$, $\tau = P\hat{\beta}$, $\tau_\delta = P\hat{\gamma}$ and $\tilde{p} = N_p\hat{p}$ where P is the stress interpolation function, the choice of which is described in [8], and N_u, N_p and B_u are as described in [14]. After substituting the interpolations and following the procedure outlined in [17] and considering a harmonic solution, we arrive at the following form of the equation,

$$\left[K_{uu}\right]\hat{u} + \left[K_{up}\right]\hat{p} = \left[f_u\right] \qquad (21)$$

where

$$\left[K_{uu}\right] = -\omega^2 \int_\Omega \rho N_u{}^T N_u d\Omega + \left[G\right]^T \left[H\right]^{-1} \left[G\right], \qquad (22)$$

$$\left[K_{up}\right] = \int_{\Gamma wet} N_u{}^T \hat{n} N_p d\Omega, \qquad (23)$$

$$\left[f_u\right] = \int_\Gamma N_u{}^T \bar{t}\, d\Gamma. \qquad (24)$$

where H and G are as described in [15], and ω is the frequency of harmonic vibration. The fluid domain is modeled using the linearized Reynolds equation given by

$$\frac{h_0^3}{12\mu_{\mathrm{eff}}}\left(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}\right) = \frac{h_0}{P_{\mathrm{a}}}\frac{\partial P}{\partial t} + \frac{\partial H}{\partial t} \qquad (25)$$

Using the process outlined in [14] we arrive at the following discretized form of Eqn. (25)

$$\left[K_{pp}\right]\hat{p} + \left[K_{pu}\right]\hat{u} = 0 \qquad (26)$$

where

$$\left[K_{pp}\right] = \frac{h_0}{12\mu_{\mathrm{eff}}} \int_{\Gamma_{wet}} B_p{}^T B_p d\Gamma + \frac{j\omega h_0}{P_{\mathrm{a}}} \int_{\Gamma_{wet}} N_p{}^T N_p d\Gamma, \qquad (27)$$

$$\left[K_{pu}\right] = j\omega \int_{\Gamma_{wet}} N_p{}^T N_{u_z} d\Gamma. \qquad (28)$$

and N_p, N_{u_z} and B_p are as described in [14]. Now, combining Eqns. (21) and (26) we get the coupled form:

$$\begin{bmatrix} K_{uu} & K_{up} \\ K_{pu} & K_{pp} \end{bmatrix} + \begin{bmatrix} \hat{u} \\ \hat{p} \end{bmatrix} = \begin{bmatrix} f_u \\ 0 \end{bmatrix} \qquad (29)$$

Implementation of Squeeze film module

Following the implementation architecture discussed in this paper, we discuss, as a representative example, the implementation of our squeeze film analysis module into an existing commercial FEA suite, i.e. NISA [16] . The implementation architecture is shown in Figure 7.

As a first step we did a 'gap' analysis where we identified the additional information needed for squeeze film analysis that is not already a part of NISA input. Thus, an additional input GUI screen with squeeze film parameters, air gap, air viscosity, ambient pressure, frequency range of operation was designed. The NISA suite generates a raw data file in a particular format based on input from user. With our special requirements, two data files in NISA specific format gets created. A parser program written in 'C' language was developed to convert the NISA raw data files into formats compatible with our FORTRAN analysis module. As the current NISA version does not allow the choice of "face id" selection by the user for denoting the face subject to squeeze film pressure, the logic was incorporated in the parser. The nodal connectivity from NISA had to be converted to the connectivity logic used in our analysis module, the conversion logic was also built into the parser.

We have incorporated a special feature "node of interest" , wherein the NISA GUI was modified to allow the use to select a particular node of choice for which nodal displacement data will be generated. The output from our module consists of nodal solutions for pressure and displacement which may be visualized using NISA post processing capabilities. A special feature "frequency sweep" which is incorporated in our squeeze film module allows for a tabular output of nodal displacement, squeeze film damping and stiffness forces and the corresponding frequency used in the computation. The data is output in a tabulated format so as to allow the use to further plot frequency response graphs or force vs frequency plots as maybe desired. The user may also compute stiffness and damping coefficients from the displacement and the force values computed at each frequency as follows: $(K = \frac{F_s}{u_z}, C = \frac{F_d}{u_z})$ where 'F_s' is the spring force, 'F_d' is the damping force and 'u_z' is the 'z' direction displacement. Figure 7. shows the process schematic for implementation of the squeeze film module into NISA.

Example

We present a test case to validate of our squeeze film solver implemented in NISA. We model a cantilever resonator and compare the first three Q factors with that from published literature. We choose to model a Si, cantilever beam as described in [21]. The simulation parameters are shown in Table 3. The beam is meshed with a converged mesh of (N_x = 40, N_y =6, N_z = 4) elements. The simulations are run for the frequencies between 1e4 Hz to 1e5 Hz in small incremental steps of 1e3 Hz. The vertical displacement 'u_z' for the tip node of the beam is noted for the range of frequencies. The corresponding value of velocity is obtained as $V_{tip} = frequency * u_z$. From the plot of normalized velocity (with input voltage) Vs frequency the Q factor is obtained using 3dB method. The computed Q factor is compared with reported values from experiments and from ANSYS [21] (See Table 4). Thus we see our squeeze film module computed Q factor compares well with experimental and numerical data from published literature. Figure 8, shows the post-processing capabilities of NISA for visualization of pressure field distribution.

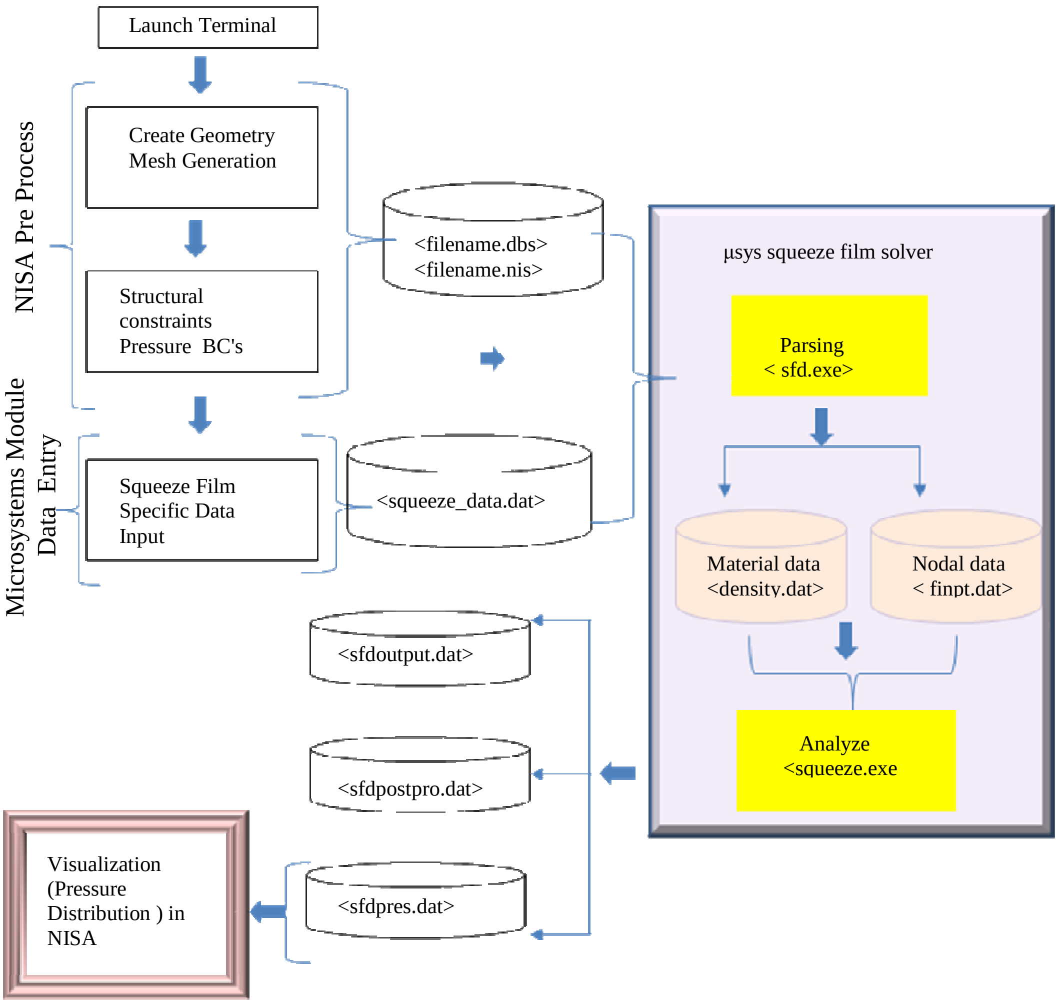

Figure 7. Squeeze film analysis module in NISA

Simulation Parameters	**Values**
Young's Modulus (Si)	160GPa
Density	2230 Kg/m^3
Poisson's Ratio	0.22
Density (air)	1.2Kg/m^3
Viscosity	1.8e-05 Ns/m^2
Air Gap	1.4 µm
Length	350 µm
Breadth	22 µm
Thickness	4 µm
Actuation Voltage	1.5 Volts

Table 3: Simulation parameters for squeeze film test case

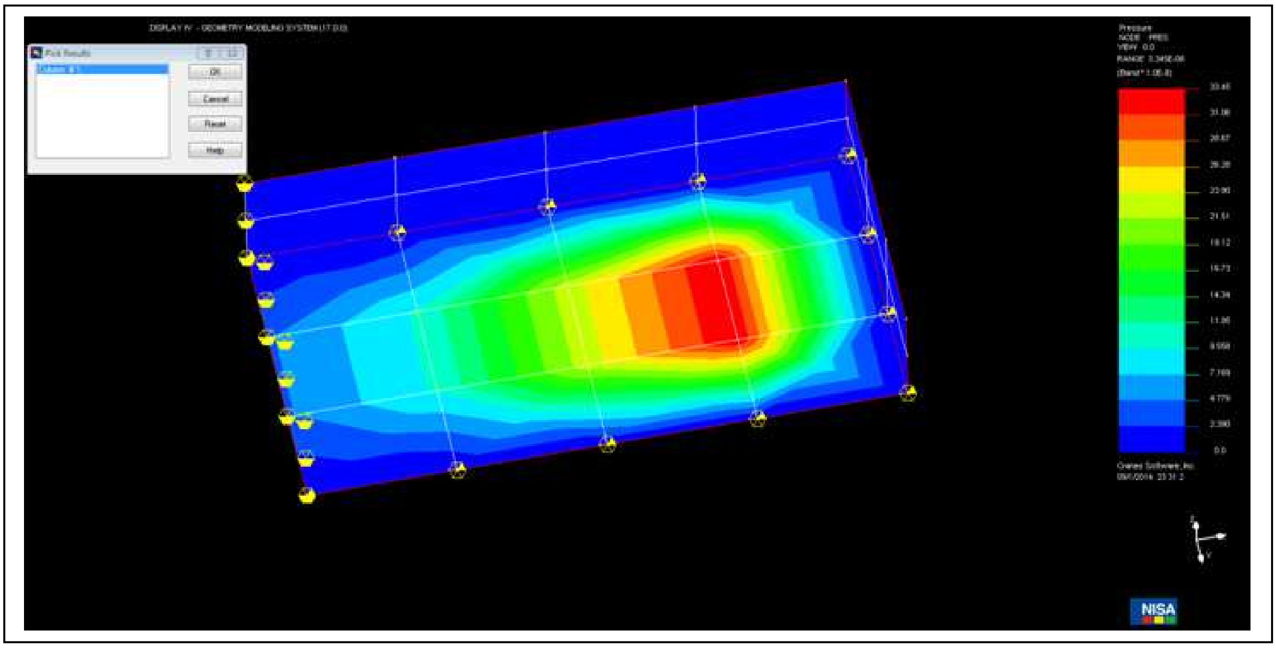

Figure 8. Squeeze film pressure distribution (on the lower surface of a cantilever) visualization in NISA

Q-NISA	Q-Exp	Q-ANSYS
1.13	1.20	1.11

Table 4: Q factor from 1st mode of a cantilever due to squeeze film

Conclusions

We described the development of hybrid finite element-based direct solution strategy in software μsys, which is capable of doing multi-physical computational analysis of microsystems. The novel features of μsys are the use of hybrid finite elements which alleviates certain short comings of conventional finite elements, and the monolithic implementation of governing equations. Implementation and working of two coupled modules, coupled structure-electrostatics and coupled squeeze film are discussed using pre- and post-processing capabilities of NISA. Currently, the major focus is on the development of analysis module of μsys and using other commercial pre- and post-processing capabilities through appropriate data parsing. Development of post-processing tool of μsys is also underway.

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