

Cross-links:

Aptamer Biosensors

Development of
Microbalance Array/
Mass Spectrometry

Biomechanical Modeling

The group 'Modeling' continued the work on mathematical models based on the Finite Element Method for a Love wave acoustic sensor, biosensor, which is under development at caesar. The sensor stands for the determination and selection of small amounts of biomolecules in biological solutions. The operating principles of the biosensor are described in the annual reports from 2000 and 2001.

The mathematical model of the biosensor consists of equations describing a piezoelectric substrate, electrodes, a guiding layer, and a liquid that contacts the surface of the device. The equations are coupled through interface conditions and electric fields generated in the piezoelectric substrate. We consider stationary solutions provided that the sinusoidal excitations are applied. In this case, we arrive at a system of Helmholtz-type equations, which requires more advanced technique to estimate the computation accuracy than in the case of a pure elliptic system. We propose an a posteriori estimate of the accuracy of Finite Element computations. This estimate can be adopted in a natural way to reduced two-dimensional models obtained via averaging either over lateral or transversal dimensions.

The direct simulation of three dimensional models is limited by the very restricted capacity of computational resources (WorkStations SUN-ULTRA60) being at our disposal at the moment. The realization could be possible on an advanced PC-cluster or several PC-clusters. We have started the development of a parallelization technique that provides the distribution of the computational work both inside a single cluster and between several clusters. The parallelization inside a single cluster is based on the domain decomposition (see Fig. 1). The original domain is divided into several sub-domains on which matrices typical for FE-method (mass, stiffness, etc) are assembled. The FE-program FelICs we use supports the identification of degrees of freedom at the intersection points, which reduces the computation of the global matrix to the summation of the partially assembled matrices.

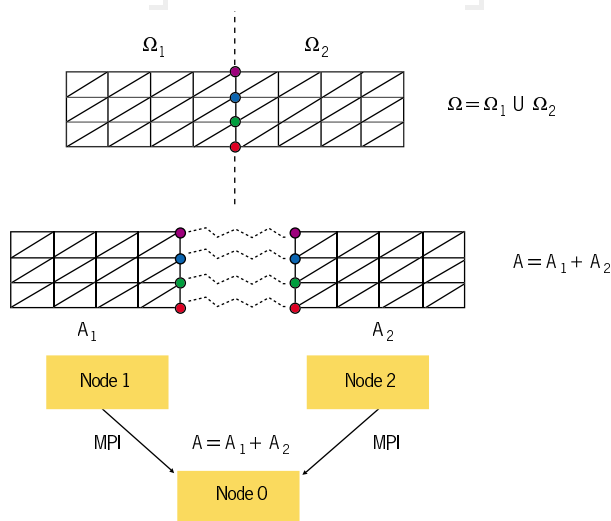


Figure 1: Illustration of the domain decomposition technique.

The parallelization between clusters is based on a structure decomposition of the problem. Navie-Stokes equations for the fluid are assumed to be solved on one cluster whereas piezoelastic equations for the solid part are being solved on the another one (Fig. 2). The matching should hold on the interface between the liquid and solid parts. This type of the interface is very hard to treat because the displacements in the solid part and the velocities in the fluid must be matched. The matching method is based on the minimization of a residual using a gradient descent method where the derivatives of the solution with respect to a coupling variable are computed through appropriate conjugate equations. Such a method requires an intensive data transfer within one solution step in time. We suppose that the communication between the clusters will be realized using MPI- and MetaMPI-protocols (Fig. 3).

Cooperation:
 University of Bonn

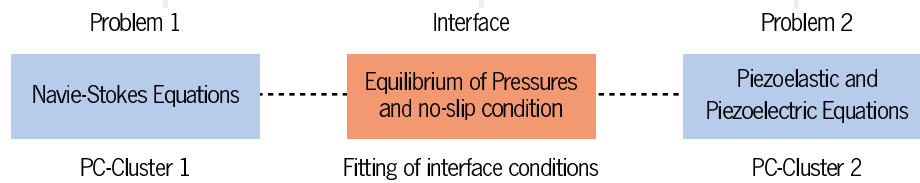


Figure 2: Structural decomposition of the problem.

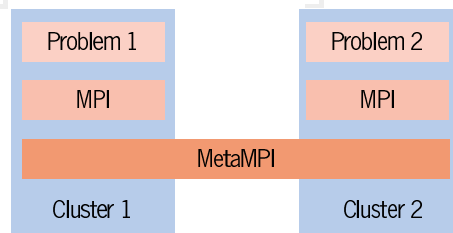


Figure 3: Parallelization between clusters.

The parallelization of FeliCs has been done for Work Stations SUN-ULTRA60 connected by a local Fast Ethernet line. Fig. 4 shows a simulation performed with a high resolution using the parallelization for a reduced 2D model obtained via the transversal averaging.

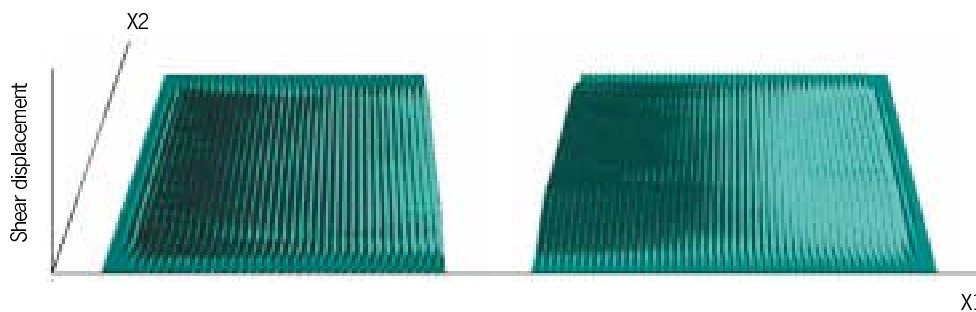


Figure 4: Fragment of the biosensor surface.