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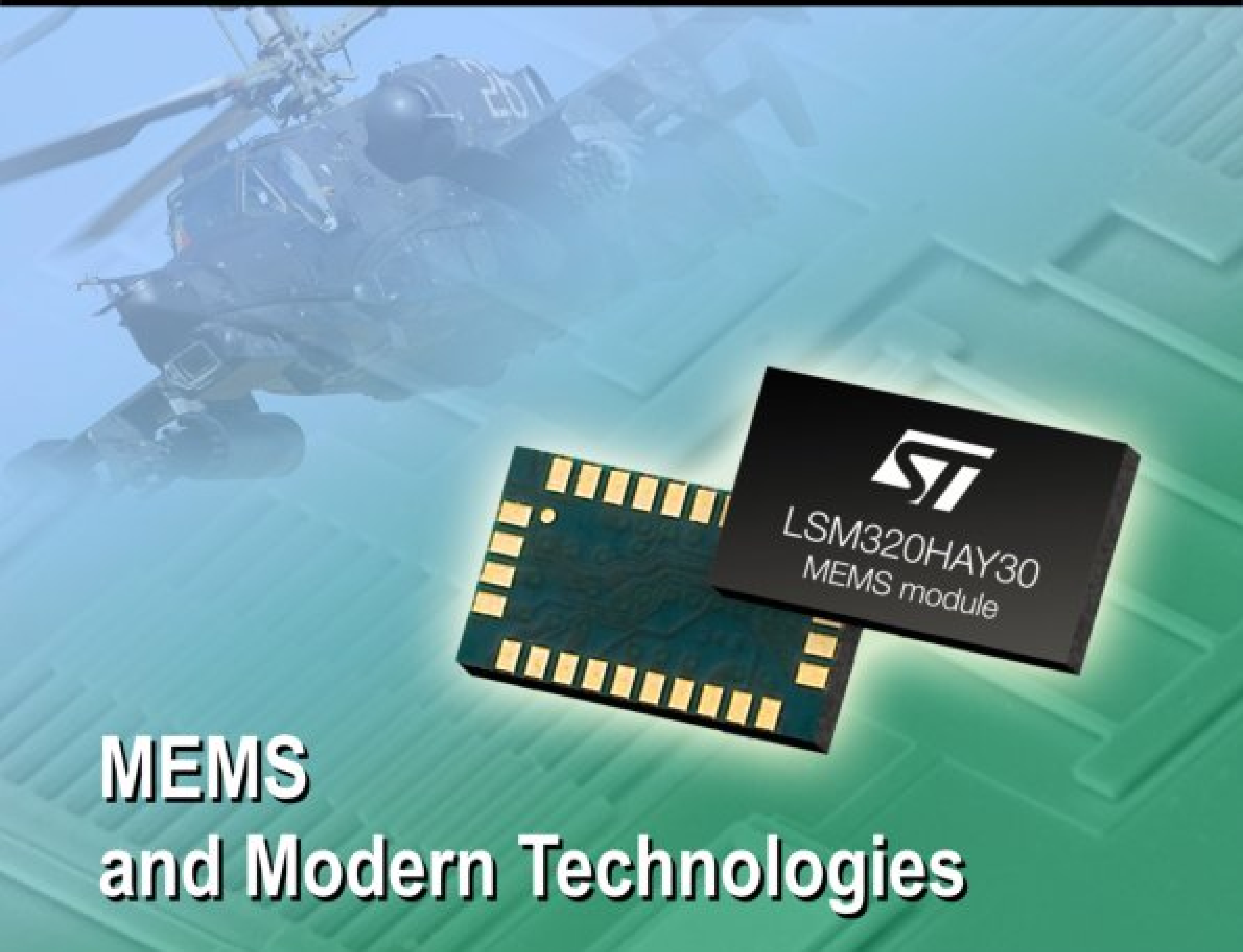

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Sensitivity Analysis of Piezo-electric Devices to Perturbed Boundary Conditions

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Abstract: The Rayleigh-Ritz method found its use in multiple branches of science and engineering. It is one of the successful variational methods for finding an approximated solution to a boundary value problem. In this paper we derive the integral functional for the Rayleigh-Ritz method for application to piezo-electric devices. A similar mathematical procedure results in a reciprocity relationship between two solutions of a piezo-electric device. The reciprocity relationship is applied to a sensitivity analysis of a piezo-electric device with perturbed boundary conditions. The connection between the theory of self-adjoint operators and the presented methods is discussed. *Copyright © 2012 IFSA.*

Keywords: Piezo-electric structures, Self-adjoint operators, Rayleigh-Ritz method.

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1. Introduction

The methods of electro-mechanical modeling discussed in this paper are well established, but currently documented approaches to similar problems in piezo-electric device analysis rely on the Lagrangian variational formalism which does not provide the desired closed form relationship for a frequency domain analysis. If one is interested in frequency stability of a piezo-electric device, the methods presented in this paper seem to have an advantage over Lagrangian methods.

If we are working with a lossless piezo-electric system that has a discrete set of mechanical modes, it is natural to consider the principle of conservation of energy. We can say that such a physical system is described as a boundary value problem in terms of the Hamiltonian "energy functional". In more general terms this Hamiltonian can be represented by a special family of differential linear operators, namely self-adjoint or Hermitian operators. Eigen-values of such operators have real values and the eigen-functions are orthogonal to each other, in respect to a defined inner product. More on the theory of self-adjoint operators can be found in [2]. One should expect a connection between basic dynamic equations for loss-less piezo-electrics and self-adjoint operators.

It is worth mentioning that Hamiltonians as self-adjoint operators found use in a theory of quantum mechanics. Quantum mechanics offers bra-ket notations for states of the Hamiltonian system. We can borrow these notations to establish one important relationship between eigen-values and eigen-functions. These notations are not specific to quantum mechanics; they can be applied for the description of piezo-electric loss-less devices. The advantages of bra-ket notations over explicit expressions for operations are its compact form and independence from the particular basis. The action of Hamiltonian operator on a ket eigen-state can be written as $\hat{H}\left|\Psi\right\rangle = \lambda\left|\Psi\right\rangle$. Here lambda is an eigen-value or energy of the Hamiltonian for a given eigen-state. Taking the inner product, we can re-write this relationship in a following form

$$\lambda = \frac{\left\langle \Psi \right| \hat{H} \left| \Psi \right\rangle}{\left\langle \Psi | \Psi \right\rangle} \tag{1}$$

In practice, Eq. (1) turns into an integral functional. There are two main results presented in this paper. First, we establish the integral relationship, equivalent to Eqn. (1), for a piezo-electric system. Integration by parts is the key to the mathematical procedure. It brings boundary conditions into an integral functional formulation for eigen-values. In general, integration by parts is used in the theory of self-adjoint operators to verify if differential operator satisfies the conjugate condition. A conjugate operator acts on braeigen-state as $\left\langle \Psi \right| \hat{H}^* = \lambda^* \left\langle \Psi \right|$, where the asterisk represents the conjugation operation.

In addition, the same mathematical procedure can be expanded to get an integral reciprocity relationship between two solutions. One of the solutions can represent the mode of the original system and another solution can represent the perturbed mode due to a change in boundary conditions. This result is applied to the following discussion of the frequency stability of piezo-electric sensors.

2. Theory

2.1. Basic Equations

The response of piezo-electric material is governed by a set of basic electro-elastic equations. Here we have a set of mechanical dynamic equations and an electrostatic equilibrium equation:

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ik}}{\partial x_k} + f_i . \tag{2}$$

$$\frac{\partial D_i}{\partial x_i} = q. \tag{3}$$

A set of constitutive piezo-electric equations:

$$\sigma_{ik} = C_{iklm} \upsilon_{lm} - e_{l,ik} E_l \tag{4}$$

$$D_i = \varepsilon_{ik} E_k + e_{i,kl} \upsilon_{kl} . \tag{5}$$

The relationships between the strain tensor and mechanical displacements and another relationship between electric field and potential:

$$\upsilon_{ik} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_i} + \frac{\partial u_i}{\partial x_k}\right) \tag{6}$$

$$E_i = -\frac{\partial \varphi}{\partial x_i}., \tag{7}$$

where:
ρ – material density;
q – free charge density;
f_i – component of mechanical body force;
σ_{ik} – stress tensor;
υ_{ik} – strain tensor;
u_k – component of displacement;
C_{iklm}, $e_{i,kl}$, ε_{ik} – material property tensors;
D_i – component of dielectric displacement vector;
E_i –component of electric field, φ – electric potential.

We need to satisfy boundary conditions on a surface S:

$$u_i(S) = U_i \tag{8}$$

$$\sigma_{ik}(S)n_k = F_i \tag{9}$$

$$\varphi(S) = V_S \tag{10}$$

$$D_i n_i = Q(S), \tag{11}$$

where:
n_i – outer unit normal to the surface;
$Q(S)$ – surface density of free charge;
U_i – mechanical displacement at the surface;
F_i – component of surface force;
V_S – surface potential.

2.2. Integral Functional

We arrive at the integral relationship, similar to Eq. (1), if we follow a few simple steps. Let us multiply the equation of motion by displacement and the electrostatic equation by potential and integrate over the volume V of the device. All the amplitudes here are real valued.

$$\int_V \rho \ddot{u}_i u_i dV = \int_V \frac{\partial \sigma_{ik}}{\partial x_k} u_i dV + \int_V f_i u_i dV. \tag{12}$$

$$\int_V \frac{\partial D_i}{\partial x_i} \varphi\, dV = \int_V q\varphi\, dV. \tag{13}$$

Integration by parts leads to:

$$\int_V \frac{\partial \sigma_{ik}}{\partial x_k} u_i dV = \int_S u_i \sigma_{ik} n_k dS - \int_V \sigma_{ik} \frac{\partial u_i}{\partial x_k} dV = \int_S U_i F_i dS - \int_V \sigma_{ik} \upsilon_{ik} dV \quad . \tag{14}$$

$$\int_V \frac{\partial D_i}{\partial x_i} \varphi \, dV = \int_S \varphi D_i n_i dS - \int_V D_i \frac{\partial \varphi}{\partial x_i} dV = -\int_S Q V_S dS + \int_V D_i E_i dV. \tag{15}$$

Combining integral relationships and applying constitutive Eqs. (4), (5) we get:

$$\int_V \rho \ddot{u}_i u_i dV = -\left(\int_V C_{iklm} \upsilon_{lm} \upsilon_{ik} dV + \int_V \varepsilon_{ik} E_k E_i dV \right) + \left(\int_V f_i u_i dV + \int_S U_i F_i dS + \int_V q \varphi \, dV + \int_S Q V_S dS \right). \tag{16}$$

If the displacement *u* describes a harmonic displacement, we can time average over the period *T* of oscillation in the right and left hand side of integral relationships Eq. (16).

$$\frac{1}{T} \int_0^T \left(\int_V \rho \ddot{u}_i u_i dV \right) dt = -\omega^2 \left\langle \int_V \rho u_i u_i dV \right\rangle, \quad \omega = 2\pi f = \frac{2\pi}{T}. \tag{17}$$

The oscillating frequency can be expressed as

$$\omega^2 = \frac{\left\langle \int_V C_{iklm} \upsilon_{lm} \upsilon_{ik} dV \right\rangle + \left\langle \int_V \varepsilon_{ik} E_k E_i dV \right\rangle - \left(\left\langle \int_V f_i u_i dV \right\rangle + \left\langle \int_S U_i F_i dS \right\rangle \right) - \left(\left\langle \int_V q \varphi dV \right\rangle + \left\langle \int_S Q V_S dS \right\rangle \right)}{\left\langle \int_V \rho u_i u_i dV \right\rangle}. \tag{18}$$

Here we found the relationship that is similar to Eq. (1). The inner product is defined in the denominator of Eq. (18). The Hamiltonian term is in the numerator. Frequency squared plays the role of the eigen-value.

We can identify time averaged electro-elastic potential energy *Π*:

$$\Pi = \left\langle \frac{1}{2} \int_V \left(C_{iklm} \upsilon_{lm} \upsilon_{ik} + \varepsilon_{ik} E_k E_i \right) dV \right\rangle, \tag{19}$$

The work *W* of external forces and charges:

$$W = \left\langle \int_V \left(f_i u_i + q\varphi \right) dV \right\rangle + \left\langle \int_S \left(Q V_S + U_i F_i \right) dS \right\rangle. \tag{20}$$

Frequency in these notations takes on a form:

$$\omega^2 = \frac{2\Pi - W}{N}, \quad N = \left\langle \int_V \rho u_i u_i dV \right\rangle. \tag{21}$$

Eq. (21) can be a starting point for a Rayleigh-Ritz minimization method. For examples on application of the Rayleigh-Ritz method, see e.g. [2]. This equation can be used for the formulation of parametric models for the Bias and Scale Factor of piezo-electric sensors.

2.3. Reciprocity Relationship and Sensitivity Analysis

Here we will outline time-independent perturbation methods applied to piezoelectric devices. We assume that the dielectric tensor ε_{ik} is symmetric and magneto-optics effects are ignored.

If we solve for the dynamic system with certain boundary conditions, we can use a set of eigen-function solutions or modes as a bias set and find corrections to these solutions in the case of small boundary load changes.

As a first step in the sensitivity analysis, we consider two different displacement solutions. Those solutions correspond to two different surface distributions of surface forces and charge; otherwise all material properties stay the same. Using steps similar to the previous section we can get the following relationship:

$$\int_V \rho\left(\ddot{u}1_i u2_i - \ddot{u}2_i u1_i\right) dV =$$
$$\left(\int_V \left(f1_i u2_i - f2_i u1_i\right) dV + \int_S \left(U2_i F1_i - U1_i F2_i\right) dS\right) - \left(\int_V \left(q1\,\varphi2 - q2\,\varphi1\right) dV + \int_S \left(Q1\,V2_S - Q2\,V1_S\right) dS\right), \quad (22)$$

This relationship can be compared to *Lorentz Reciprocity* in electrodynamics.

If we take *u1* as the perturbed harmonic solution and *u2* as a mode of the unperturbed system, we can re-write the above expression for surface boundary conditions in the right hand side as:

$$\left(\omega_2^2 - \omega_1^2\right) \int_V \rho\, u1_i u2_i \, dV = \int_S \left(\left(U2_i F1_i - U1_i F2_i\right) + \left(Q2\,V1_S - Q1\,V2_S\right)\right) dS, \quad (23)$$

In the following discussion, an upper index in round brackets is used to annotate the mode. It is convenient to use complex amplitudes to take into account in-phase and quadrature vibrating components. For example, modal displacement can be represented as

$$u_i^{(m)}(t) = \frac{1}{2} u0_i^{(m)} e^{-i\omega_m t} + \frac{1}{2}\left(u0_i^{(m)}\right)^* e^{i\omega_m t}, \quad (24)$$

where:
$u0_i^{(m)*}$ – complex conjugate of $u0_i^{(m)}$.

There are second order effects in displacement that can be very important to piezo-electric device operation. For example, for a double ended tuning fork, as the beam vibrates, the effective beam length gets longer. This exerts a force on the beam support proportional to the square of tine displacement. This means that static offset and the second harmonic as well as the fundamental are present in a beam support structure. For now, we'll omit the second order terms and discuss a linear theory of piezoelectric devices.

We are looking for a perturbed system solution as a linear superposition of modes of the unperturbed system:

$$u1_i = \sum_m b_m u0_i^{(m)} \quad (25)$$

$$\varphi1 = \sum_m b_m \varphi0^{(m)} \quad (26)$$

$$\upsilon 1_{ik} = \sum_m b_m \upsilon 0_{ik}^{(m)} \tag{27}$$

$$\sigma 1_{ik} = \sum_m b_m \sigma 0_{ik}^{(m)} \tag{28}$$

$$E1_i = \sum_m b_m E0_i^{(m)}, \tag{29}$$

where:

b_m –constants to be determined.

$$\int_V \rho u1_i \left(u1_i\right)^* dV = N_0 \sum_m \left|b_m\right|^2, \quad \sum_m \left|b_m\right|^2 = 1. \tag{30}$$

The normalization constant N_0 is the same for all the modes.

The free surface charge for a new system has a small variation in the area that is not covered by electrodes, i.e. $Q(S) = Q_0(S) + \delta Q_o$. We assume that perturbed solution is close to the nth mode, meaning that $\left|b_n\right| \approx 1$, and much bigger than the other indices.

If we substitute the complex amplitudes into Eq. (23) and collect the terms with time the varying factor $e^{i(\omega_m - \omega)t}$, where the index stands for the m-th mode, we get

$$\left(\omega^2 - \omega_m^2\right) b_m N_0 = \int_S \left(\tilde{Q}(\omega) \cdot \left(\tilde{V} 0_S^{(m)}\right)^* - \tilde{V} 1_S(\omega) \cdot \left(\tilde{Q} 0(\omega_m)\right)^*\right) dS - \int_S \left(\left(\tilde{U} 0_i^{(m)}\right)^* \tilde{F}_i(\omega) - \tilde{U} 1_i(\omega) \left(\tilde{F}_i(\omega_m)\right)^*\right) dS. \tag{31}$$

where:

The real surface force amplitude is $F(t) = \frac{1}{2} \tilde{F}_i(\omega) e^{-i\omega t} + c.c.$

The real surface potential is $V(t) = \frac{1}{2} \tilde{V}_i(\omega) e^{-i\omega t} + c.c.$

The real surface displacement is $U(t) = \frac{1}{2} \tilde{U}_i(\omega) e^{-i\omega t} + c.c.$

c.c. - complex conjugate.

This procedure is similar to the demodulation of a signal with a frequency difference harmonic. In a first approximation, if the perturbed mode is close to the n-th mode, we can say

$$\left(\omega^2 - \omega_n^2\right) \approx I(\omega_n) = \frac{1}{N_0} \left| \int_S \left(\tilde{Q}(\omega) \cdot \left(\tilde{V} 0_S^{(m)}\right)^* - \tilde{V} 1_S(\omega) \cdot \left(\tilde{Q} 0(\omega_m)\right)^*\right) dS - \int_S \left(\left(\tilde{U} 0_i^{(m)}\right)^* \tilde{F}_i(\omega) - \tilde{U} 1_i(\omega) \left(\tilde{F}_i(\omega_m)\right)^*\right) dS \right|. \tag{32}$$

It is interesting that static charges, even in the area outside electrodes, do not contribute to Eq. (32). In order to include static charges and static force loads to the frequency shifts, we need to consider nonlinear terms in displacement, proportional to the square of harmonic displacement. In that case Eq. (32) is modified by adding integrals with similar structure for second harmonic and static offset.

As a last remark on sensitivity analysis, frequency perturbation relationships like Eq. (31) for loss-less devices can be extended to perturbations causing losses on a boundary. By introducing small imaginary part to the frequency, see e.g. ref. [4], we get

$$(\omega + i\gamma)^2 - \omega_n^2 \approx (\omega^2 - \omega_n^2) + 2i\gamma\omega \approx 2\omega_n \cdot (\Delta\omega + i\gamma), \quad \Delta\omega = \omega - \omega_n. \tag{33}$$

Separating the real and imaginary parts, we find a model for the change in frequency and the half width, half maximum γ of mode resonance due to boundary conditions,

$$\Delta\omega \approx \frac{1}{2\omega_n}\mathrm{Re}(I_S) \tag{34}$$

$$\gamma \approx \frac{1}{2\omega_n}\mathrm{Im}(I_S) \tag{35}$$

where:
I_S – surface integral in the right hand side of Eq. (31).

3. Conclusion

Integral relationships for piezo-electric devices have been discussed. One of these integrals is a starting point for the Rayleigh-Ritz minimization method. It also can be used for a parametric model of the frequency of piezo-electric sensors. Another integral relationship represents the reciprocity between two solutions for the piezo electric system with different boundary conditions. The application of the reciprocity integral leads to a frequency sensitivity analysis. It has been shown that the above approach is rooted in a theory of self-adjoint operators and the principles of conservation of energy.

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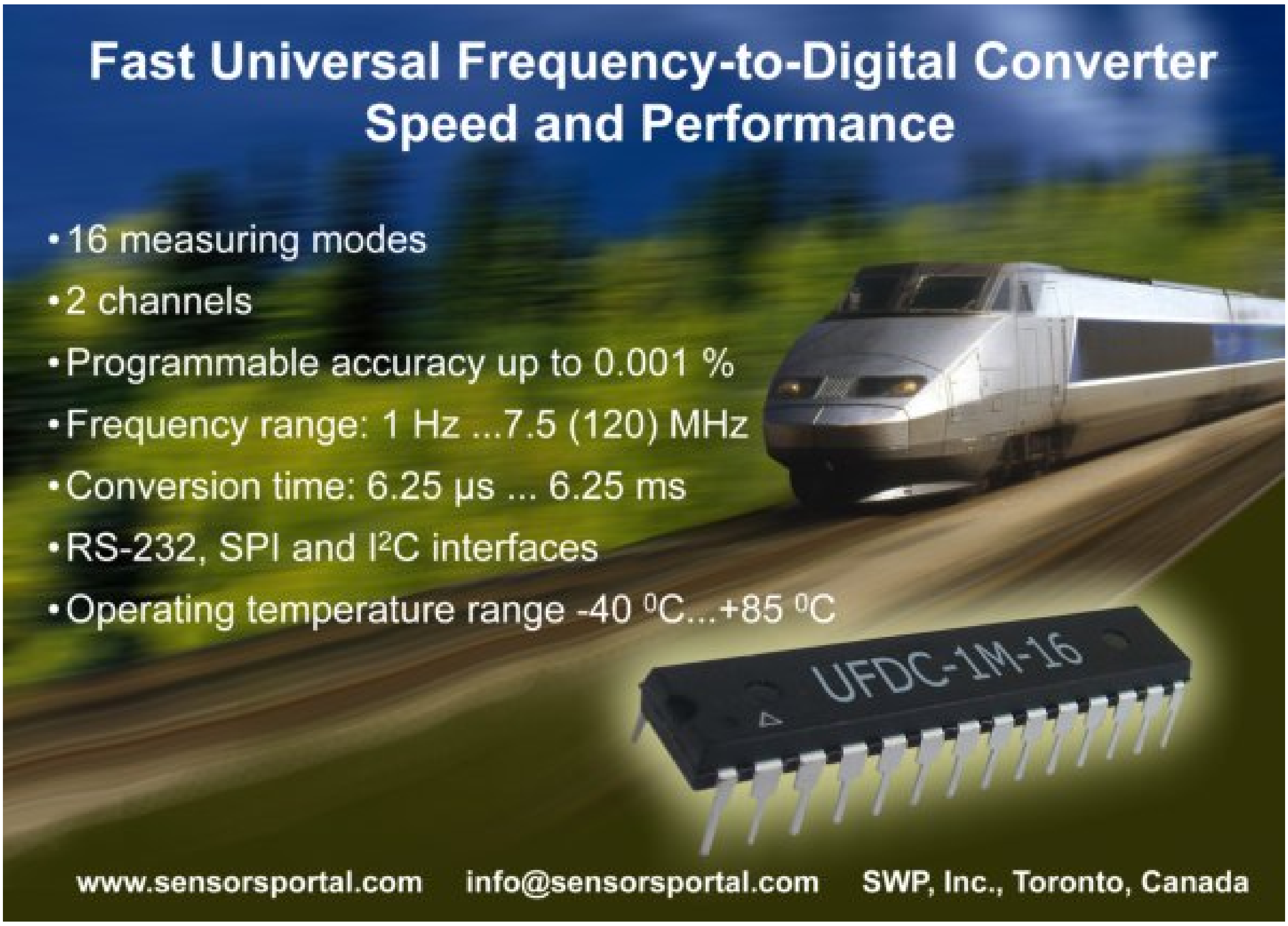

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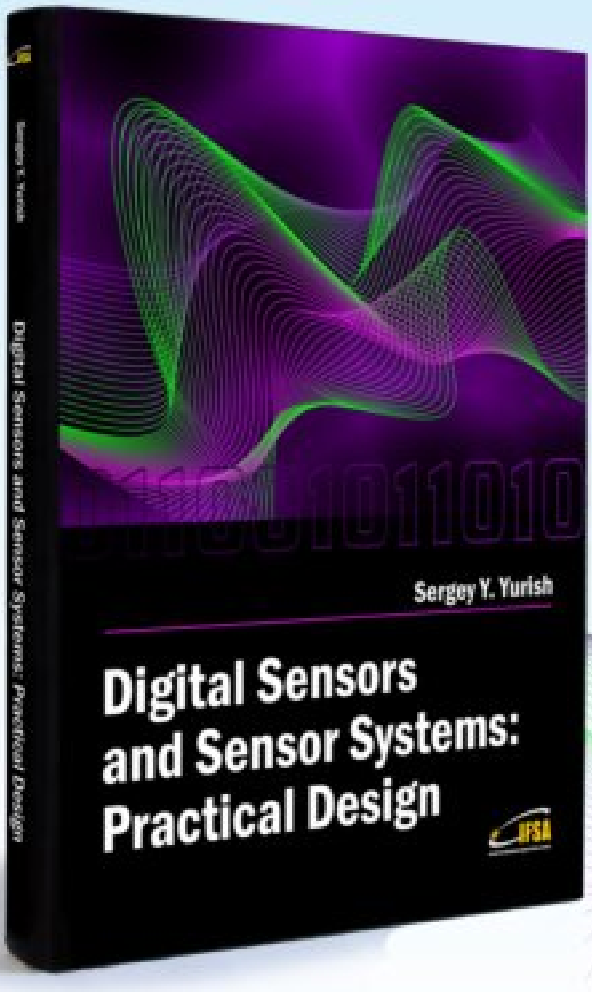

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