In such complex physical ensembles as semiconductor heterostructures the investigation of physical phenomena connected with transport of charge carries an energy is impossible without modeling of this phenomena and enhanced numerical calculations. The transport equations are nonlinear and their solution needs a special treatment. It's needs the applying of iterative methods and needs the constructing a suitable numerical schemas which guarantee stability and efficiency of solution. As we are the authors of enhanced numerical programs and we have over 30 years of experience in modeling of transport and fluctuation phenomena in semiconductor heterostructures we know what to do to make our programs to have wider applications and work more efficien then now. These change are necessary due to necessity of analyzing and designing the new types of infrared detectors manufactured by applying the heterostructures and super lattices.

That is why the essential goal of this project is to improve and develop a wide spectrum of models of physical phenomena connected with detection of electromagnetic radiation in semiconductor devices based on epitaxial layers manufactured by using MOCVD and MBE technology. These models include transport phenomena as well as the fluctuation phenomena being the sources of noise current in detectors. They will be elaborated by applying the basic postulates and rules of the thermodynamic of non-equilibrium processes. As a results we will derive the expressions for non-equilibrium statistical distribution functions. These functions depend on temperature gradient and gradient of electrochemical potentials. We derive them by using our original postulated variational principle for steady state condition, which gives the results more general and more exact than in the standard approach by solving the Boltzmann kinetic equation. We will formulate the balance equations of the energy of localized states, such as ionized impurities and structural defects to calculate their own electrochemical potentials. The resulting theoretical model will provide us tools which can be used to design of very complex infrared detectors by using computer programs.

.The second crucial goal of the project is to improve of our, already existing, computer programs. The balance equations, as well as the Poisson equation used in the description of complex transport phenomena are non-linear differential equations, and thus they can be effectively solved only by numerical iterative methods. In this point of the project we plan to develop numerically stable iterative schemas simultaneously limiting the number of iterations by a self-acting choice of the numerical steps of time and the steps of spatial coordinates. All these changes will significantly limit the time of calculations. We also will improve our computer program used for numerical modeling of fluctuation phenomena. In the modified version we would like to take into consideration the tunneling effect as well as the surface G-R processes as additional noise sources.

We will verify the correctness of our models and numerical programs with experimental data For these verifications , the available in literature experimental data will be considered as well as a suitable HgCdTe heterostructures will be created by using MBE technology in University of Western Australia in Perth (professor Faraone's group) and MOCVD technology in MUT-Vigo System joint laboratory. We have cooperated with Faraone's group for many years , and lately in project Harmonia DEC-2013/08/M/ST7/00913. I am manger of this project and it will be finished in August 2016. They are strongly interested to continue cooperation.

As a finalt result of the project, we will obtain an effective numerical tool for the designing of infrared detectors fabricated from strongly non-homogeneous structures. We will be able to investigate complex photoelectrical and fluctuation phenomena in heterostructures by applying advanced numerical calculations. The applicability of our programs will be increased due to the control of the stability and convergence of the iterative schemes use as well as due to the application of the new iterative schemes for boundary conditions. It is worth to stress that the effective numerical modeling of infrared detectors will enable to find optimally designed solutions without expensive and time-consuming experimental investigations. We hope that the successful realization of the project will give the chance for commercialization of our simulators. Offered commercially simulators very often cost more than the expenses connected with proposed project.