Mathematical models as research data in numerical simulation of opto-electronic devices

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***Abstract*—Mathematical models are the foundation of numerical simulation of optoelectronic devices. We present a concept for a machine-actionable as well as human-understandable representation of the mathematical knowledge they contain and the domain-specific knowledge they are based on. We propose to use theory graphs to formalize mathematical models and model pathway diagrams to visualize them. We illustrate our approach by application to the stationary one-dimensional drift-diffusion equations (van Roosbroeck system).**

I. Introduction

The numerical simulation of optoelectronic devices is characterized by (possibly huge amounts of) data and software used for its generation. In order to ensure reproducibility as well as re-usability of the scientific results appropriate options for their storage and long-term accessibility of the involved research data are required.

The *numerical data* is generally recognized as research data in the usual sense, which stimulated the setup of data repositories and related information services such as DataCite [1] or RADAR [2]. However, a valid interpretation of the numerical data and the reproducibility of the scientific results require the corresponding *software* to be available. Hence, software is increasingly recognized as research data by scientific communities and funding agencies, so information services for mathematical software such as swMath [3] emerge.

II. Mathematical models as research data

Still, this is not enough to fully characterize the research data in areas of *mathematical modeling and simulation* (MMS) that has been utilized to achieve the scientific results because numerical data and the corresponding software can only be correctly interpreted and used if the corresponding *mathematical models* are explicitly linked to both. Therefore [4], [5] propose to categorize mathematical models as the third pillar of research data in MMS beside numerical data and software.

However for models, finding an appropriate representation is far less obvious than for numerical data and software. The current practice is a mixture of mathematical formulae and natural language in scientific publications. This (rigorous, but) informal approach creates ambiguity, potential incompleteness of the presentation, less reproducibility and often "re-invention of the wheel".

In particular, this representation is not suited for the creation of a "model repository" in analogy to those for data and software. To remedy this [6] proposes a new machine-actionable, but human-understandable representation of mathematical models that relies on the physical quantities that are described in the model and the relations between them (laws, constitutive equations). These are then represented in a flexiformal representation using the OMDoc/MMT language [7], [8]. In this paper, we review the flexiformal model representation developed in [6] and demonstrate its usefulness on an example of the van Roosbroeck model.

III. Model Pathway Diagrams

In [6] we developed a diagrammatic representation of mathematical models, the **Model Pathway Diagram** (MPD), that reflects its inner (physical) structure. In an MPD the physical quantities are depicted as circles with their physical notations as labels connected by the physical laws in a rectangle labeled with the respective equations.

As an example we consider the stationary van Roosbroeck model describing the semi-classical transport of electrons and holes in a self-consistent electric field using a drift-diffusion approximation. The van Roosbroeck model is the standard model to describe the current flow in semiconductor devices at macroscopic scale and widely used for the numerical simulation of optoelectronic devices covering LEDs, lasers and solar cells. The MPD of a unipolar version of van Roosbroeck model is shown in Fig. 1.

In the context of perturbation theory in quantum field theory the usefulness of diagrammatic representations, notably Feynman diagrams for complex physical phenomena is well-established. We hope that MPDs similarly provide generally an easy access to inner structure of complex mathematical models as its topological structure reflects important properties of the subsystems. For instance, the loop of the nonlinear Poisson equation in Fig. 1 reflects the self-consistency of the electric field.

We have formalized the underlying physics of the van Roosbroeck model in an OMDoc/MMT theory graph [7], [8] using the MPD in Fig. 1 as a guide; see [9]. As OMDoc/MMT is machine-oriented, we support directly MMS workflows via the the MMT system [10]. Our formalization of the unipolar stationary one-dimensional van Roosbroeck system is significant first step towards the formalization of the mathematical

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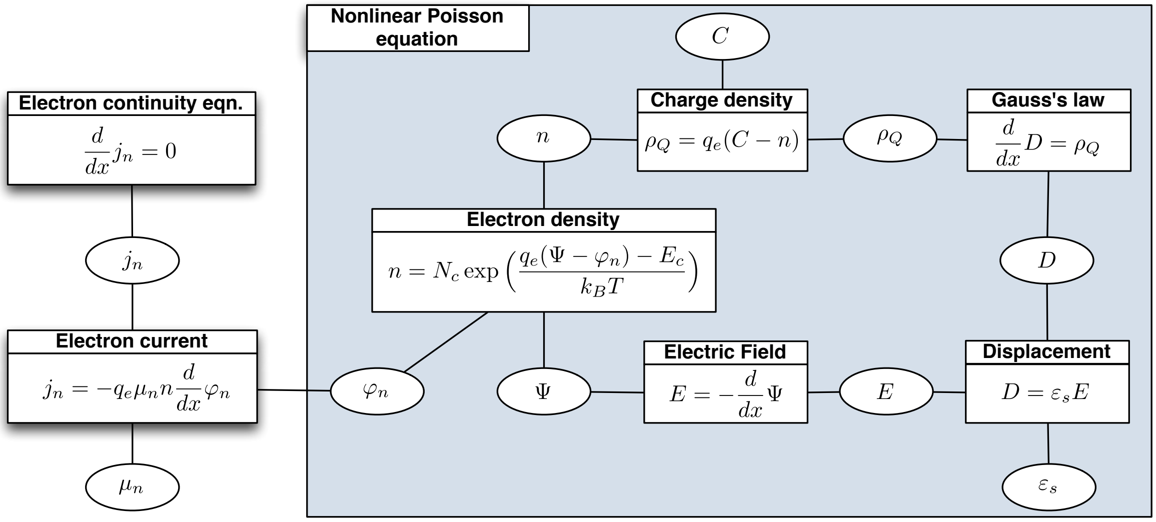

Fig. 1. Model Pathway Diagram (MPD) of unipolar van Roosbroeck system in one-dimension. One observes the nonlinear Poisson equations complex on the right (highlighted with blue color) and the carrier transport complex on the left. The loop structure of the nonlinear Poisson equations reflects the self-consistency of the electric field, whereas the transport complex reveals a tree-like structure. (Material) parameters of the van Roosbroeck model appear as leafs of the MPD such as the doping profile C, the permittivity ε_s or the electron mobility μ_n. For simplicity the representation of the boundary conditions have been omitted as well as some quantities, e.g. the density of states N_c or the temperature T.

models relevant for numerical simulation of optoelectronic devices. We started a collection effort for MPDs on [11].

IV. Benefits of a flexiformal representation of mathematical models

The representation of mathematical models as outlined in the preceding section enables the unique identification of mathematical models, the automatic derivation of relationships between them and a modular creation of new models from existing (then sub-)models.

As a first concrete tool, we have created a special theory graph viewer that given such a MMT model representation shows the graph as a MPD – just as in Fig. 1. In the MPD viewer all nodes and edges are clickable and produce interactive HTML5 renderings of the formal contents.

Additionally, OMDoc/MMT have a well-established interface to a semantically enhanced Version of TEX, i.e., sTEX(semantic TEX/LATEX) that can be used to write semantically enhanced articles and papers, that directly refer to the database of mathematical models. From these we can generate HTML5/Web documents which can be instrumented with semantic services like the ones above.

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