Rules of thumb for creating useful reduced models: the case study of nanopores

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"All models are wrong, but some are useful." said George Box in 1976. How true it is! This presentation is about how we can create useful reduced models. In a complex many-particle system, by reduced model we mean that some of the degrees of freedom are modeled explicitly, while some of them are modeled implicitly. The explicit degrees of freedom are the important ones that we handle with explicit particles in the model and in the associated computer simulations. The implicit degrees of freedom are the less important ones that are modeled by implicit response functions. By useful reduced models we mean models that can predict and explain the relationship between the input and output variables of a device. We call this relationship the device function. The art of creating good reduced models lies in distinguishing between the important and unimportant degrees of freedom. Here we present rules of thumb that we can apply in a procedure of constructing reduced models of nanopores that facilitate the controlled transport of ions through a membrane. This system is a device of basic importance both in biology (ion channels) and in technology. Controlling the ion transport depends on molecular level phenomena so using a molecular model is essential. In the case of nanopore, we balance between the need for molecular description (more detail) and the need for efficient computation of device behavior (less detail). This balance results in the useful reduced model. We show, for example, that basic device functions can be understood and reproduced by using the implicit-water framework where the effect of water molecules on ions are described by two response functions: their screening effect on electrostatic forces is described by a dielectric constant of a dielectric continuum, while their frictional effect on moving ions is described by a diffusion coefficient. Results are shown for selective ion channels and rectifying nanopores.

REFERENCES

[1] D. Boda, M. Valiskó, D. Gillespie. Modeling the device behavior of biological and synthetic nanopores with reduced models. *Entropy*, 22 (2020) 1259.

FIGURES

Figure 1: A typical reduced model that can reproduce device behavior.