Computational Methods on Multiscales
Before the works of Kurt Gödel, the idea of a complete formalization and axiomatization of all mathematics, introduced by David Hilbert at the beginning of the 20th century (Hilbert’s program), was predominant in the area of mathematics. Mathematics was supposed to be described within the framework of a “logical calculus”, a formal, non-contradictory and closed system of axioms. The basic idea of this formalization was to derive all mathematical theorems, which are recognized as true, by logical deduction from some prefixed axioms. In essence, this means that all true mathematical theorems can be generated by a systematic, algorithmic process.

In the 1930s Kurt Gödel managed to show that Hilbert’s idea was doomed by proving that any formal logical calculus, which is sufficiently complex, i.e. which contains theorems on the natural numbers (such as number theory), contains an infinite number of theorems which can neither be proved nor disproved within this logical system. Such theorems are called undecidable. In other words, Gödel managed to prove that any sufficiently complex logical system based on a set of axioms is incomplete, and he showed this explicitly for the axioms of number theory. As a consequence, for example, there exists no algorithm, which is capable of solving any complex mathematical problem, and there is no algorithm that can be used to proof the correct functioning of a different algorithm.

Roughly during the same period of time, Allan Turing provided a simple definition of a machine, called Turing machine, that can execute an algorithm. The concept of a Turing machine was developed in order to provide a fundamental notion of algorithmic computability. Despite its simple construction, a Turing machine is universal, that is, any intuitively calculable function, i.e. a function that can be solved using an algorithm, can be calculated by a Turing machine. This is underpinned by Church’s thesis which states that the Turing machine is an adequate model for computability that includes all other possible models.

The formal developments in mathematical logic and the formalization of a notion of algorithm and computability were accompanied by two major
physical theories, discovered and formulated during the first quarter of 20th
century: Quantum Theory and the Theory of Relativity. Based on the duality
of particle and wave concepts as fundamental principles of physical theory,
Quantum Theory changed profoundly the general notion of what is to be con-
sidered reality in physical theories. With the extension of Quantum Theory to
Relativity Theory and to the quantization of fields, along with the application
of symmetry principles of group theory, it became possible to describe three of
the four known fundamental interactions within one theoretical system. The
mathematical ontology of modern physics is thus based on symmetries, fields,
and particles.

On the other hand, with the discovery of the Theory of Special Rela-
tivity, it became evident, that the distinctive status of inertial systems is
not only valid for the mechanical equations of Newton’s theory, but for all
physical processes. The mathematical framework which is used in this the-
ory is based on the invariance of the spacetime interval in Minkowski space
for all observers in inertial systems. Each observer uses his own system of
synchronized clocks to measure time and length intervals. The Theory of
General Relativity extends this invariance of a general line element to ob-
servers, which are not in an inertial frame of reference. This is a major dif-
ference to pre-relativistic Newtonian theory according to which there exists
a global coordinate time which is the same for all observers. As a conse-
quence of this invariance principle, one has to formulate physical theories
in tensorial form which ensures their invariance against arbitrary non-linear
transformations between frames of reference. This naturally leads to the use
of curvilinear coordinate systems and to a concept of non-Euclidean, curved
spacetime in which the components of the fundamental metric tensor are
coordinate dependent. Einstein’s field equations of General Relativity The-
ory (GRT) provide the connection between the sources of mass and electro-
magnetic fields given in the energy-momentum tensor, and the metric tensor
which is a tensor of rank 2. The differential geometric concepts on which
GRT is based were developed in mid 19th century by Carl Friedrich Gauss,
Janos Boliay and N. Iwanowitsch Lobatschewski, and were finally general-
ized to a theory of manifolds by Bernhard Riemann in his inaugural speech
in 1856, when he introduced a generalized concept of space, which allowed
for a separate treatment of the underlying space (topology) and its geo-
metry. This concept was later further formalized using basic set theory. These
mathematical formalizations allow for a deeper understanding of different
concepts, or levels of space, depending on the amount of algebraic structure
that is provided on the respective level. In this sense, Relativity Theory is a
framework theory which provides the basic spatio-temporal structure for the
natural sciences, and theories formulated using this spacetime structure in
Riemannian geometry are considered to be more fundamental than those that
are not.

With the development of the first electronic computers in mid 1940s, a
new way of performing scientific research became accessible, namely the use
of computers to investigate in detail the behavior of $N$-particle systems, with differential equations too complex to be solved analytically. This development of computational science has not come to an end, and the scope of possible applications is steadily increasing with the discovery of new efficient algorithms and the steady increase of hardware capabilities.