PhD thesis proposal

"Robust discretization for coupled mechanical systems based on generalized geometry"

Supervision: Vladimir Salnikov and Aziz Hamdouni
Location: LaSIE, La Rochelle University, France
Keywords: differential geometry, mechanics, geometric integrators, fluid–structure interaction.

Practical details

Application procedure: The application including a CV, a motivation letter and eventually recommendation letter(s), is to be sent to vladimir.salnikov@univ-lr.fr and aziz.hamdouni@univ-lr.fr.
Deadline for application: 15.05.2019
Contract: 36 months starting in October 2019; salary: $\sim$ 1400 €/month (slightly depending on the fiscal situation); a right for some optional teaching load.

Description of the project

Supervision and team

The PhD student will be supervised by Vladimir Salnikov (CNRS Researcher) and Aziz Hamdouni (Professor), both from La Rochelle University, France.
He/she will be working in the Laboratory of Engineering Sciences for Environment (LaSIE) in the La Rochelle University (`https://lasie.univ-larochelle.fr/`), team "Mathematical and Numerical Methods" (`https://lasie.univ-larochelle.fr/E1-M2N`).

Main topic

In this thesis we would like to contribute to the development of mathematical and numerical tools, appropriate for modelling of multi-scale, multi-physics and strongly coupled systems. More precisely, we plan to study geometric structures that appear naturally for such problems, and numerical methods that "respect" these structures. We also pay attention to efficient implementation of the designed algorithms. Our range of applications is motivated by mechanical problems, and fluid–structure interaction in particular, but the framework is not limited to those.

Motivation

Even if nowadays it is relatively easy to have access to serious computational resources, development of efficient methods remains a real challenge. Let us just name an example in this context:
In the fluid–structure interaction problem, the main difficulty is the size of data one needs to handle. On the one hand, one needs to take into account the geometry of the interface between the solid and the fluid, thus, introduce a very fine mesh. It is also important to have good discretization in time to capture the dynamics and especially deformations of the solid, that can influence the spacial mesh as well. On the other hand studied systems are usually very large, if one compares them with the scale of the interface and deformations. One thus needs to work with enormous mass of information, that results in algorithmic and technological issues, meaning that the"brute-force" approach of increasing the size of the calculator is not efficient. For this mentioned case, as well as for many others, one needs reliable numerical schemes, preferably with reasonable computational cost and necessarily scalable.

State of the art

For *conservative mechanical systems* the Hamiltonian/Lagrangian formalism gives a rather convenient framework for analysis of qualitative properties (like for example integrability or stability). From the numerical point of view, the integrators called *symplectic* ([1, 2]) exist for some decades already – they permit to control energy conservation, and they are frequently used for instance in Molecular Dynamics. The idea behind the method is to construct a discretization that will automatically preserve a symplectic structure – this will guarantee the conservation of a Hamiltonian function that oscillates in a small neighborhood of the value of total energy of the system. The phenomenon persists even for large time intervals, in contrast to other numerical schemes even of higher order ([3]). The Lagrangian counterpart of this construction is related to integrators called *variational* ([4]).

A lot of works have shown that numerical schemes that mimic physical properties of differential equations are more robust. The challenge is then to understand what mathematical structures one needs to consider while discretizing the equations to guarantee the conservation of physical quantities. Numerical schemes constructed in this manner are often called *geometric integrators*, since the mathematical structures behind come from differential or algebraic geometry. In present days, there is a number of works related to methods preserving geometric structures, like symplectic, Lie symmetries ([5]), first integrals that result from the Noether's theorem. More generally, geometric integrators have been shown ([6, 3]) to be more robust for some PDEs, this is a very important result, saying that these schemes can be good candidates for simulation of large volumes mentioned in the introduction.

When one considers the generalization of the above discussion to systems with *dissipation*, *interaction with the environment*, or *coupled* systems the situation is less clear both from the geometric and numerical points of view. One of possible convenient formalisms is related to so-called *port–Hamiltonian systems* ([7]), that is with additional terms corresponding to interactions with other systems, internal or external dissipation, It appears that the analogue of symplectic/Poisson geometry in the port–Hamiltonian case is related to (almost) *Dirac structures* ([8]). Those have also turned out to be useful for numerical methods appropriate for the mechanical systems with constraints ([9], [10]), important in particular in robotics. In the context of partial differential equations the situation is less straightforward as well. Among the appropriate structures it is worth mentioning *multi-symplectic forms* ([11]), *contact geometry* and *jet spaces* ([12]) – those permit to define the symmetries and conserved quantities as well as to treat partial derivatives morally as independent variables and thus regain the intuition from the finite-dimensional case.

Candidate and tasks

We are searching either for a candidate specializing in mathematics (differential geometry or mathematical aspects of theoretical physics), capable to understand problems coming from mechanics and having some knowledge about numerical methods, or for a candidate specializing in mechanics having a solid general mathematics background and a capacity to master geometric topics. He/she will work on some concrete examples of mechanical systems within the approach described in the introduction. Ideally, that would include the "full cycle" of formalizing the model, spelling-out the geometric counterpart of the governing differential equations, designing and implementing the appropriate numerical methods. Some programming skills are certainly useful but not strictly mandatory.

References

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