M2 internship proposal 2023–2024

Title: Reliable numerical integration

Topics: symbolic and numeric algorithms, reliable computing, integrators

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Context

The MAX team is searching for PhD candidates on the themes of the ANR “NODE” project. The present M2 internship proposal allows applicants to familiarize themselves with these themes. Upon successful completion of the internship, there will be an opportunity to pursue with a PhD. The ANR NODE project provides funding for two PhD grants.

Description

How to predict planetary motion, the spread of an epidemic, or the evolution of a chemical reaction network? Here are some of the many problems that can be modeled by ordinary differential equations (ODEs). The resolution of such equations has a long history and remains an important problem in science and technology.

Consider a system of differential equations of the form

$$f'(z) = \Phi(f(z)), \tag{1}$$

where $f: \mathbb{R} \to \mathbb{R}^n$, $\Phi: \mathbb{R}^n \to \mathbb{R}^n$, and an initial condition is provided at $z_0 \in \mathbb{R}$. The numeric integration of such a system is a widely studied problem in numeric analysis. The function Φ can usually be an arbitrary smooth function and the integration is typically done with machine precision. Runge–Kutta schemes are the most common workhorse in this situation [2, 3, 12]. Systems and libraries like MATLAB [14], DIFFERENTIALEQUATIONS.JL [13], or SUNDIALS [4] offer extensive suites of solvers adapted to various kinds of problems and accuracy requirements.

This internship concerns the certification problem: given $\varepsilon > 0$ and $z_1 \in \mathbb{R}$ such that (1) can be integrated on $[z_0, z_1]$, how to compute an approximation $\tilde{f}(z_1)$ of $f(z_1)$ with $|\tilde{f}(z_1) - f(z_1)| \leqslant \varepsilon$. There exist several software packages for this task [1, 9, 11], most which implement certified numerical schemes that are based on Taylor series expansions. For efficiency reasons, one might prefer certified counterparts of more traditional Runge–Kutta integrators.

The aim of the present internship proposal is the development and implementation of reliable counterparts of traditional Runge–Kutta schemes. Implementations will be done in C++ within the MATHEMAGIX libraries; see http://www.mathemagix.org.

One popular approach to reliable computation is to use interval or ball arithmetic [10, 5, 8, 7]. This amounts to systematically replace any floating point approximation $\tilde{x}$ of a real number x by an interval $[c-\varepsilon, c+\varepsilon]$ that is certified to contain the exact value x. There is a trade-off between the efficiency of operations for this kind of arithmetic and the quality ε of the error bounds [6]. We aim to develop interval and ball versions of Runge–Kutta schemes that are both efficient and accurate (i.e. the produced error bounds ε are as small as possible).

We seek for excellent candidates with a background both in mathematics and computer science. Applicants will be required to have knowledge in complex analysis, differential equations, algorithms. Skills in computer science will be needed to achieve efficient implementations in C++.

Bibliography

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