INTEGRATION OF PDEs USING RESERVOIR COMPUTING

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Número máximo de estudiantes: 2

Artificial Intelligence is a strategic line for many institutions and companies for the next decade, as it offers many new and powerful development and innovation opportunities in very different fields.

One such technique is known As Reservoir Computing [1].There have appeared recently in the literature a good number of relevant papers under this title [2,3], which successfully apply Neural Networks and Deep Learning to the integration of non-trivial differential equations in partial derivatives. We here propose to apply the above mentioned tools to the study of the Schrödinger equation, both in the time-independent and time-dependent versions, for its interest in quantum problems. In particular, we propose application in Quantum Chemistry and Quantum Chaos, in which the group leader has extensive experience.

We look preferably for candidates with knowledge or interest in Python programming techniques and also an interest in theoretical aspects.

Along the work he/she will apply our computer programs to integrate the Schrödinger equation using Deep Learning and Reservoir Computing techniques to study quantum mechanically the vibrations of small floppy polyatomic molecules with chaotic classical behavior. We will also explore if time permits other application and try to characterized the networks used in the calculations from the point of view of the field Complex Networks, trying to understand the origin of their good performance.

[1] Y. LeCun, Y. Bengio, and G. Hinton, *Deep Learning*, Nature **521**, 436 (2015).
[2] J. Pathak, B. Hunt, M. Girvan, Z. Lu, and E. Ott, *Model-Free Prediction of Large Spatiotemporally Chaotic Systems from Data: A Reservoir Computing Approach,* Phys. Rev. Lett. **120**, 024102 (2018).
[3] L. Domingo and F. Borondo, *Deep Learning Methods for the Computation of Vibrational Wavefunctions,*Commun. Nonlinear Sci. Numer. Simulat. **103**, 105989 (2021).

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