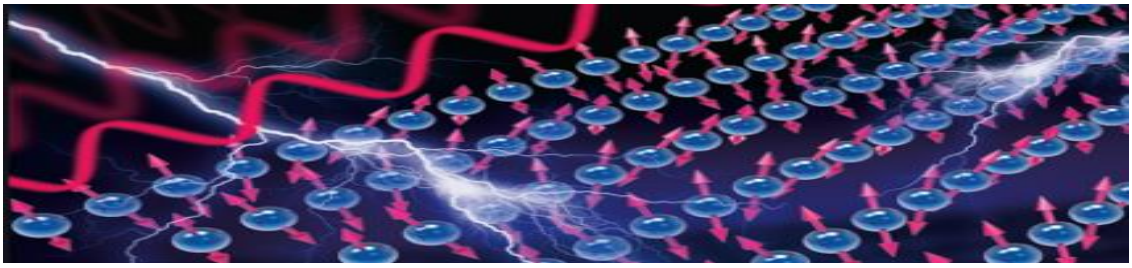
SPILADY - A Spin-Lattice Dynamics Simulation Program

Developed at CCFE under EUROfusion Enabling Research grant, this Spin-lattice dynamics simulation software generalise molecular dynamics to the case of magnetic materials and can simulate dynamic evolution involving non-collinear fluctuations of magnetic moments and translational motion of atoms on a million atom scale. These simulations have been applied to a variety of systems, such as iron thin films, the treatment of self-diffusion in iron and dynamic magneto-caloric effects, and can provide key informations on the materials such as thermodynamics, superconductivity, phase transitions, thermal conductivity, and thermal expansion

Description of the technology

The technology is a spin-lattice dynamics code intended to serve as an introductory computer simulation tool for undergraduate students, scientists, researchers, and others familiar with molecular dynamics. The approach that was followed during the development of SPILADY involved introducing a number of new software architecture and data structure concepts, that differ from those used in other implementations of spin-lattice dynamics, including earlier numerical realizations of the method.

The approach followed during the development of SPILADY involved introducing a number of new software architecture and data structure concepts, that differ from those used in other implementations of spin-lattice dynamics, including own earlier numerical realizations of the method. Applications of the method include atomistic models for defects, dislocations and surfaces in magnetic materials, thermally activated diffusion of defects, magnetic phase transitions, and various magnetic and lattice relaxation phenomena.



The code is parallelized in coordinate and spin spaces, and is written in OpenMP C/C++ for CPU and in CUDA C/C++ for Nvidia GPU implementations. Temperatures of atoms and spins are controlled by Langevin thermostats. Conduction electrons are treated by coupling the discrete spin-lattice dynamics equations for atoms and spins to the heat transfer equation for the electrons.

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission

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Innovation and advantages of the offer

Understanding lattice dynamics is important for a number of key applications. The propagation of sound waves in crystals are a practical example of the role of lattice dynamics, as also is the interaction of materials with light. For example, the absorption of certain frequencies in the infra-red spectral region is directly due to the existence of specific lattice dynamics motions. Lattice dynamics also gives us properties such as thermodynamics, superconductivity, phase transitions, thermal conductivity, and thermal expansion.

Non-fusion Applications

Spin-lattice dynamics simulations have been applied to a diverse range of applications in fission and fusion, and beyond. For example, simulations explain the anomalous variation of elastic constants, lattice structure, vacancy formation and migration energy near the Curie temperature. Other applications explored using spin-lattice dynamics simulations include the correlated dynamics of magnetic moments in thin films, ultrafast demagnetization of materials by a laser pulse, and ultra-high frequency magnetic refrigeration

EUROfusion Heritage

SPILADY (pronounced as [spileidi]) is a computer program written at the Culham Centre for Fusion Energy from March 2014 to July 2015. The development and release of this SPILADY program has been made possible through the support provided by a EUROfusion Enabling Research grant WP14-ER-01/CCFE-02 "Dynamic Evolution of Non-Equilibrium High Temperature Thermodynamic Properties of Magnetic Metals". The work was carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and from the RCUK Energy Programme.

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