The *spin-transport* documentation

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Abstract

The *spin-transport* software (GitHub) is for the dynamic simulation of bulk spin transport—diffusion and separation—in solid media. The project is open-source and still in development.

Contents

1 Installation

This repository contains the (developing) open-source code for simulating bulk spin transportmdash;diffusion and separationmdash;in solid media. Multi-spin-species and magnetic resonance simulations are in development.

This is a [Python](https://www.python.org/) and [FEniCS](https://fenicsproject.org/) project. FEniCS is used to numerically solve the spin transport governing partial differential equations.

End users of this project write Python code to interface with FEniCS.

One must first have a working installation of FEniCS. This README assumes the use of [Docker](https://www.docker.com/) for installation, which is documented [here](http://fenics.readthedocs.io/projects/containers/en/latest/).

Then [clone](https://help.github.com/articles/cloning-a-repository/) this repository to the host machine.

The FEniCS docs have a section on [workflow](http://fenics.readthedocs.io/projects/containers/en/latest/work$_flows.ht$
$nixsystem, thefollowingmaybetheeasiest$.

With the cloned `spin-transport` repository as your working directory, create a link in your path to **spin-transport**'s `fenics` executable bash script.

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"'bash ln fenics /usr/local/bin "'

Now a FEniCS Python script `foo.py` can be started with the command `fenics foo.py` **from the host** instead of manually starting it from a Docker container. This has several advantages, including that there is no need to move scripts into the container and that the complicated syntax need not be remembered.

To verify that everything is installed correctly, run the Poisson equation demo `ft01_poisson.py` ([source](https://fenicsproject.org/pub/tutorial/html/._ftut1004.html))inyourcontainer.

If you installed the `fenics` bash script per the instructions above, you can use the following command (working directory: `spin-transport`).

"'console $fenicsft01_{p}oisson.py$"'

If everything is working fine, the output should look something like the following.

"'console $fenicsft01_{p}oisson.pyCallingDOLFINjust-in-time(JIT)compiler, thismaytakesometime.---Instant : compiling---CallingFFCjust-in-time(JIT)compiler, thismaytakesometime.CallingFFCjust-in-time(JIT)compiler, thismaytakesometime.CallingFFCjust-in-time(JIT)compiler, thismaytakesometiDegreeofexactsolutionmaybeinadequateforaccurateresultinerrornorm.CallingFFCjust-in-time(JIT)compiler, thismaytakesometime.CallingFFCjust-in-time(JIT)compiler, thismaytakesometiin-time(JIT)compiler, thismaytakesometime.CallingFFCjust-in-time(JIT)compiler, thismaytakesometiin-time(JIT)compiler, thismaytakesometime.error_{L}2 = 0.00823509807335error_{m}ax = 1.33226762955e-15$"'

The directory `spin-transport/poisson` should have been created and should contain two files: `solution.pvd` and `solution000000.vtu`. These files contain the solution data.

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This project stems from a collaboration among three institutions:

[Cornell University (http://www.cornell.edu/),

[Saint Martin's University (https://www.stmartin.edu/), and the

[University of Washington (http://www.washington.edu/).

The lead contributor to this project is [Rico Picone, PhD](http://ricopic.one) of Saint Martin's University, co-PI on the ARO grant. Other contributors include [John Marohn, PhD](http://marohn.chem.cornell.edu/) (Cornell, PI), John A. Sidles, PhD (Washington), Joseph L. Garbini, PhD (Washington), and Corinne Isaac (Cornell).

2 Short theoretical introduction

References

[1] Jean-Philippe Grivet. Simulation of Magnetic Resonance Experiments. *American Journal of Physics*, 61(12):1133–1139, 1993.