

# Continuum multi-physics modeling with scripting languages: the `Nsim` simulation compiler prototype for classical field theory.

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**Abstract** We demonstrate that for a broad class of physical systems that can be described using classical field theory, automated runtime translation of the physical equations to parallelized finite-element numerical simulation code is feasible. This allows the implementation of multiphysics extension modules to popular scripting languages (such as Python) that handle the complete specification of the physical system at script level. We discuss two example applications that utilize this framework: the micromagnetic simulation package `Nmag` as well as a short Python script to study morphogenesis in a reaction-diffusion model.

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# 1 Introduction

The approach towards multiphysics simulations chosen for the Nsim compiler prototype resolves the fundamental conflicts that arise in multiphysics simulations in a different way than other multiphysics packages. We hence discuss some general concepts related to continuum multiphysics first before we give an overview over the structure of Nsim and its intended uses.

## 1.1 General aspects of multi-physics simulations

When physical phenomena have to be studied quantitatively that involve complex geometries, numerical methods that discretize space – such as finite element based techniques

– often are the method of choice. As sufficient computing power to study continuum phenomena only became available within the last few decades, continuum simulations are a comparatively recent activity within physics. Not surprisingly, the design of computational simulation packages more or less followed the subject classification of physics, i.e. there are specialist packages for electromagnetism, fluid dynamics, elastomechanics, etc. As the simulation of different physical phenomena often requires very different numerical techniques, this certainly is justified, but to the physicist who is more interested in the system he would like to study than in the technology that enables the analysis, this creates an awkward problem: Often, interesting phenomena involve the interplay of effects of very different nature. To a scientist or engineer who is studying such situations in systems with geometries that are simple enough or allow justifiable approximations so that they can be handled with pen and paper alone, this is not much of a problem, as she has learned to use the analytic framework to combine quantitative descriptions that originate from different branches of physics: the discipline sub-classification is mostly perceived as a tool to organize articles in a library. In computer simulations of continuum phenomena, however, this does easily become a problem, as simulation codes that deal with different phenomena (and usually are fairly complex) are not as easily combined as the underlying equations. This has led to the concept of ‘Multi-Physics simulations’ – a curious term that is perhaps difficult to make sense of without some understanding of this context, in particular the artificial entrenchment of physics sub-disciplines imposed by software requirements that only exists in such a form in computational physics.

As ‘continuum multi-physics’ phenomena evidently are technically very important – many a device works by utilizing different physical effects, e.g. converting one form of energy into another – this gave rise to ‘Multi-Physics Simulation Packages’ that have the capability to combine continuum models from different physics sub-disciplines into unified simulations. While the existing packages are invaluable for the analysis of a large variety of commercially as well as research relevant systems, their design usually is strongly governed by the idea to support the most well established, most mature, physical models. To the research physicist working e.g. in a field where general consensus on the most appropriate phenomenological model has not been reached yet (such as, for example, micromagnetic-spintronic interactions), this results in a serious dilemma: On the one hand, domain-specific simulation packages cannot be used as the system to be studied involves the interplay of different effects. On the other hand, multiphysics packages usually do not support the very specialized sets of equations that are actively debated in an evolving field. The only option that often remains is to invest a large amount of programming effort to implement a new niche software framework from scratch.

Certainly, the situation would improve if casual familiarity with computer programming already sufficed to combine different sets of equations as easily as a physicist is used to doing it with pen and paper. Essentially, this means that it should be possible to specify the physics that governs a system at the level of an accessible high-level scripting language, as part of a simulation and data analysis script. This idea goes beyond what many of the more generic object-oriented multiphysics frameworks offer in that the user of the framework does not have to have expertise in object-oriented programming and software design. Technically speaking, the main difference is that the ability to specify physical equations from within a scripting language requires run-time compilation of physical equations to fast machine code, while with an ‘object oriented library framework’, this translation happens in the final compilation phase that produces an executable pro-

gram. The extra degree of flexibility offered by the run-time dynamic approach precisely parallels the situation that arises when trying to answer the question ‘how can I write a program that asks the user to enter a function and then plot it’ in a language like Python and in a language like C.

## 1.2 The Nsim system

This work provides a detailed report on both the conceptual as well as implementation aspects of an automatic generic framework for the translation of classical field theory physics to parallel numerical simulation code. The user of the framework provides symbolic representations of algebraic field equations as well as differential operators which get mapped to numerical code that executes the corresponding computations. To give an example, the discretised sparse matrix operator that maps a scalar field  $\phi(\vec{x})$  to its gradient  $H_j = \frac{\delta\phi}{\delta x_j}$  gets represented by the string “-<H(j) || d/dxj phi>”.

The simulation compiler Nsim parses such expressions and uses symbolic transformations to automatically create the appropriate fast code (via specialization of closures) that populates the sparse finite element operator matrices. In a parallel computation, this code is then distributed across all nodes and used to set up the corresponding sparse matrices in parallel. Furthermore, as the numerical solution of ordinary differential equations for time integration often benefits greatly from knowledge of the system’s Jacobian (e.g. when dealing with stiff ordinary differential equations), the Nsim compiler can do symbolic transformations on the equations of motion (i.e. taking derivatives) in order to auto-generate the code needed to populate the Jacobi matrix, hence rendering the (otherwise often fairly awkward) tasks of manually writing and debugging the corresponding low-level code unnecessary.

## 1.3 Architecture overview

Figure 1 shows the different layers of the simulation framework described in this work. Level 0 represents the set of numerical libraries which provide the essential low-level functionality for parallel simulations, the most prominent ones being PETSc [1] for parallelizable sparse matrix linear algebra, ParMETIS [2] for mesh partitioning, and Sundials [3] for integrating stiff ordinary differential equations. Level 1 (“Nsim simulation compiler”) represents the core of the work described here, and (due to the need to do fast symbolic transformations) has been implemented in the Objective Caml language [4]. There is a higher-level Python [5] interface (level 2) to this Nsim library which can be used to completely specify the physics to be simulated within the Python programming language. We refer to this as the “Nsim model-builder interface”, as it will require some expert knowledge (of the Nsim notation) to be able to specify a simulation at this level.

For a given research domain, such as e.g. micromagnetism, one often observes that many groups of users (e.g. experimentalists) are mostly interested in carrying out a limited number of simulation tasks common to the field, which, however, often may use some theoretical/phenomenological models which may be far from well-established at that time. Therefore, it makes sense to implement the functionality needed to perform such numerical simulations as an application library on top of a generic field theory package. This design has been chosen for the micromagnetic simulator Nmag [6]: The Nmag package

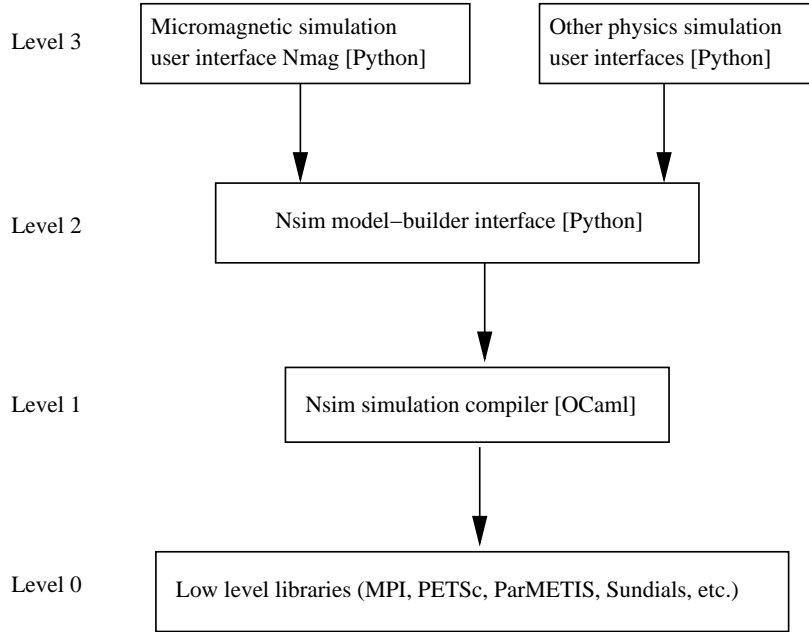


Figure 1: Overview over software layers.

is just a thin layer of micromagnetism-related definitions on top of the (level 2) `Nsim` model-builder interface that provides micromagnetic capabilities in the form of a Python extension module to the end user. The users of the (level 3) `Nmag` system need not be aware of the lower levels, and can easily combine micromagnetic computations with data analysis routines offered by other, unrelated, Python packages.

We include a brief description of `Nmag` to better illustrate how the different layers fit together, and to demonstrate their different purposes. Figure 2 shows an example `Nmag` program as end-users might write it, and figure 3 shows the simulation results.

## 1.4 Research context

The design of this framework is driven by the need to do computer simulations of the behaviour of engineered systems that involve novel combinations of physical effects. As research *by definition* often has to deal with new suggestions for model equations that try to describe physical behaviour, this situation is markedly different from the one addressed by commercial multiphysics simulation packages that face a strong incentive to only offer system components based on well-established and by now widely used theoretical models. In particular, the authors' highest priority is to provide flexibility with regard to the adoption of novel model equations.

In more detail, the aspects addressed in this work include:

- Bookkeeping infrastructure for arbitrary-rank tensorial fields (in arbitrary dimension) associated with component-dependent physical characteristics (e.g. conductive/non-conductive).

```

import nmag
from nmag import SI

# create simulation object
sim = nmag.Simulation()

# define magnetic material
Py = nmag.MagMaterial(name = 'Py',
                      Ms = SI(1e6, 'A/m'),
                      exchange_coupling = SI(13.0e-12, 'J/m'))

# load mesh
sim.load_mesh('disk.nmesh.h5',
             [('disk', Py)],
             unit_length = SI(1e-9, 'm'))

# set initial magnetisation
sim.set_m([0,0,1])

# set external field
sim.set_H_ext([0,0,0], SI('A/m'))

# integrate over time until (meta-stable) equilibrium is found
sim.relax()
sim.save_data(fields='all') # save all fields spatially resolved
                             # -> Plot on left-hand side

sim.set_H_ext([4e4,0,0], SI('A/m'))
sim.relax()
sim.save_data(fields='all') # -> Plot on right-hand side

```

Figure 2: The Nmag simulation script used to compute the data shown in figure 3. The level of computer programming skill required to write such short scripts that set up and execute basic simulations like this should be accessible to most research groups in an active field like micromagnetism. This Python program imports the Nmag library in the first line, which is the top-level user interface (level 3 in figure 1) to the Nsim simulation package.

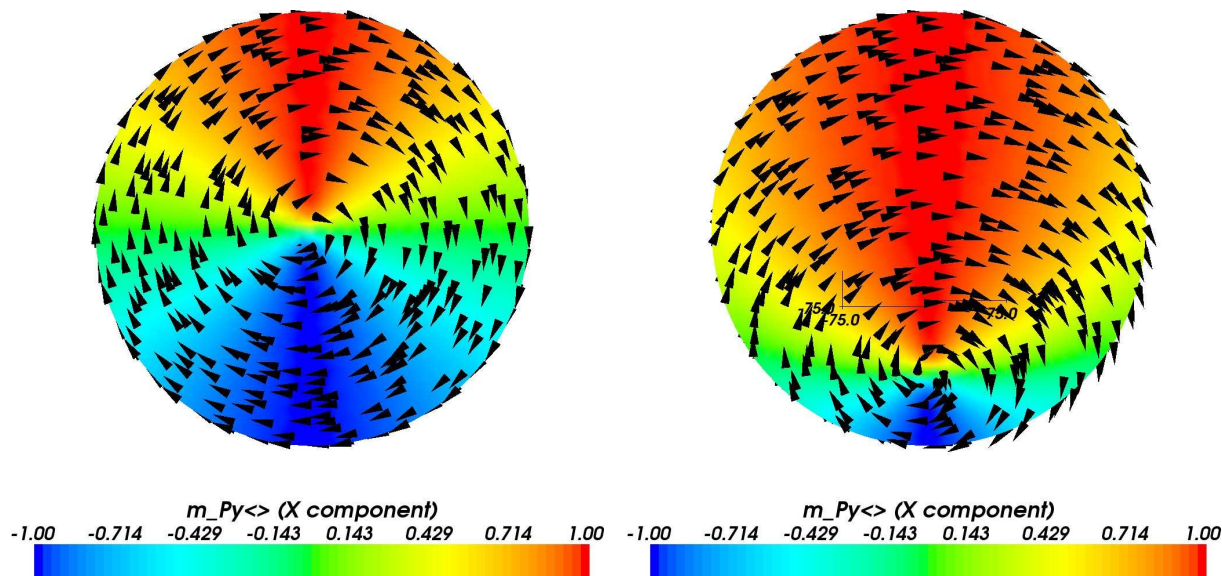


Figure 3: The results produced by the micromagnetic simulation script from figure 2

- Providing a flexible, fully scriptable end user interface towards compiled code that can be readily combined with a large collection of existing software libraries for scientific analysis (level 2), and may be used to quickly put together domain specific simulation packages (level 3).
- Automatically producing fast machine code from a symbolic representation of (potentially non-linear) physical equations that can be changed at run time (e.g. interactively).
- Embedding symbolic term transformations in a numerical simulation framework in order to automatically generate the Jacobian needed for the time integration of stiff systems.
- Relieving the user from having to deal with memory management issues.
- Psychological aspects related to how convenient different syntactic approaches towards specifying boundary conditions, equations of motion, etc. turn out to be in real use scenarios.

This work describes in detail the *prototype* (level 1) implementation of the `Nsim` simulation compiler at the time of this writing. This compiler forms the basis for the multiphysics micromagnetic simulation library `Nmag` (level 3). As some parts of `Nsim` still experience considerable evolutionary changes, this work inevitably suffers from a ‘moving target’ problem in the sense that there are some loose ends that will be addressed in the future, and that the ongoing development is driven by the input from the wider academic community.

The only spatial discretisation scheme supported by `Nsim` is finite element discretisation using unstructured simplicial meshes (i.e. tetrahedral meshes in three dimensions). While the structure of the system would support generalizations towards other methods for discretising space, this has not been implemented so far.



The outline of this work is as follows: Section 2 describes the phenomenological model that gave the original motivation for this work – micromagnetism – and some aspects of both the relevant physics and its implementation. Section 3 provides the context for the simulation compiler presented here. Section 4 explains key aspects of the model-builder interface. Section 5 then explains in detail what low level techniques are used in the prototype implementation to provide this functionality. Section 6 comments on limitations, before we summarize in section 7. Appendix A provides a complete worked out (level 2) Python example that shows how to use `Nsim` to set up a continuum physics simulation from scratch.

## 2 Motivation/Example

The scientific incentive for this work was provided by the need to implement an extensible simulation framework for computational micromagnetism that is easy to extend towards novel combinations of effects, e.g. to quantitatively study magnetoelectric, magnetothermal, and other ‘magnetism+X’ phenomena. We discuss the structure of the micromagnetic `Nsim` application, `Nmag`, in some detail in order to give an example of the techniques and approaches available to implementors of libraries that deal with other systems.

### 2.1 Micromagnetism

As mesoscale magnetism involves the interplay of a number of physical effects of very different nature yet similar strength, simulations of mesoscopic magnetization dynamics are at the same time somewhat challenging to set up (due to the amount of effort required to deal with each relevant effect separately), yet rich in interesting behaviour. It is precisely this richness in structure caused by the competition between different physical effects that makes magnetism an interesting candidate for a number of applications, first and foremost data storage utilizing hysteretic effects and multiple (thermally sufficiently stable) local energetic minimum configurations.

The selection of effects supported by a micromagnetic simulation framework is to some degree a matter of practicability and community consensus. From a condensed matter perspective, magnetism interacts with an enormously broad range of other solid state physics sectors through thermomagnetic, magnetoelastic, magnetoelectric and other effects. As a number of these offer interesting potential for novel applications: for example, new magnetic media storage devices might employ heating to above the ferromagnetic phase transition temperature in Heat Assisted Magnetic Recording (HAMR) [7] or exploit spin-polarized electric currents in novel 3d-magnetic memory (e.g. “Racetrack Memory” [8]) devices. Therefore, one would like a micromagnetic simulation framework to be extensible enough to easily accommodate such specific additional effects. If it can be designed in such a way that extensions are treated on the same footing as already existing features, then this clearly should be regarded as an important advantage.

From the perspective of using a specific challenge as guidance when devising a versatile general framework, it is important to choose a primary application that is sufficiently rich in structure to cover and test the majority of generic features required. It hence seems reasonable to expect that most problems of practical relevance to which the `Nsim` framework can be applied are structurally much simpler than micromagnetism.



We briefly describe the structure of the field theoretical model of micromagnetism as originally presented by Brown [9].

The fundamental degrees of freedom are provided by a vector field  $\vec{M}(\vec{x})$  describing the local magnetization, more precisely, the local magnetic dipole momentum density: When integrated over a region  $\Omega$  of space,  $\int_{\Omega} \vec{M}(\vec{x}) d^3\vec{x}$  gives the total magnetic dipole momentum contained in that region.

Physically, the magnitude of  $\vec{M}$  is determined by local material properties, hence constant. (At least in the commonly used zero-temperature micromagnetic model). Thus, there actually are only two dynamical degrees of freedom at every point – the direction of the magnetization vector in space.<sup>3</sup> In simulations, one hence usually prefers to take a unit-normalized field  $\vec{m} = \vec{M}/|\vec{M}|$  as the fundamental dynamic quantity.

The dynamics of the field  $\vec{M}(\vec{x})$  is governed by the so-called Landau Lifshitz and Gilbert (LLG) equation which describes the reaction of magnetization to an effective magnetic field. This equation is local and non-linear, but still polynomial in the fields involved. As  $|\vec{M}|$  is constant,  $d\vec{M}/dt$  must be perpendicular to  $\vec{M}$ , and in the simplest possible phenomenological model should be proportional to the effective magnetic field strength experienced locally. So, the most general expression possible is:

$$\frac{d}{dt} \vec{M}(\vec{x}) = c_1 \vec{M}(\vec{x}) \times \vec{H}_{\text{eff}}(\vec{x}) + c_2 \vec{M}(\vec{x}) \times \left( \vec{M}(\vec{x}) \times \vec{H}_{\text{eff}}(\vec{x}) \right), \quad (1)$$

which is just the LLG equation. The  $\vec{M} \times \vec{H}_{\text{eff}}$  term gives rise to magnetic precession, as is easily seen by noting that this is perpendicular to both  $\vec{M}$  and  $\vec{H}_{\text{eff}}$ , hence does not change the angle between  $\vec{M}$  and  $\vec{H}_{\text{eff}}$ . Precession usually dominates the motion of a magnetic moment in an external field. The other term is dissipative in nature and causes the magnetization to eventually align with the applied field.

In more systematic tensor-index notation (where we now also suppress the spatial dependency on  $\vec{x}$  and use Einstein's summation convention), this can be written as:

$$\frac{d}{dt} M_i = c_1 \epsilon_{ijk} M_j H_{\text{eff}k} + c_2 \epsilon_{ijk} M_j \epsilon_{kmn} M_m H_{\text{eff},n}, \quad (2)$$

with  $\epsilon_{ijk}$  being the fully anti-symmetric rank-3 tensor that is defined by:

$$\det(\vec{u}, \vec{v}, \vec{w}) = \epsilon_{abc} u_a v_b w_c. \quad (3)$$

While this equation automatically ensures the conservation of  $|\vec{M}|$ , in numerical simulations that use three coordinates to encode the direction of  $\vec{M}$ , rounding may cause some drift that violates this constraint. One convenient way to deal with this problem is to modify the equation of motion by adding another term which physically always is zero, but keeps numerical drift in check:

$$\frac{d}{dt} M_i = c_1 \epsilon_{ijk} M_j H_{\text{eff}k} + c_2 \epsilon_{ijk} M_j \epsilon_{kmn} M_m H_n^{(\text{eff})} + c_3 M_i (M^2 - M_k M_k). \quad (4)$$

The `Nsim` prototype exclusively employs tensor-index notation, as this is both systematic enough to be processed easily yet powerful enough to express even uncommon equations, e.g. involving angular momentum flow.

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<sup>3</sup>In group theory language one may think of this as a  $S^2 \simeq SO(3)/SO(2)$  coset model.

Contributions to the effective magnetic field strength  $\vec{H}_{\text{eff}}$  include the externally applied field  $\vec{H}_{\text{ext}}$  (which may be Earth’s magnetic field, or a field applied in a laboratory setting), the so-called ‘demagnetization field’  $\vec{H}_{\text{demag}}$  that gives the magnetic field generated in one location by the combined effects of the magnetic dipoles distributed throughout the system, as well as others that, for the purpose of magnetization dynamics, behave like contributions to the effective magnetic field, but are not linked to a true magnetic flux density. One of these is the effective magnetocrystalline anisotropy  $\vec{H}_{\text{anis}}$ : In crystals, alignment of the direction of magnetization with a crystallographic axis may be energetically favorable, and a magnetic moment starting out in a direction of non-minimal energy will precess and ring down in a way that is just equivalent to the dynamics modeled by the LLG equation with a direction-dependent effective ‘equivalent’ magnetic field strength. Physically speaking, the magnetocrystalline anisotropy arises from the coupling of spin and orbital angular momentum of the magnetic electrons, hence is a quantum effect. Another related quantum effect gives rise to a further ‘magnetic field equivalent’ contribution: The quantum mechanical overlap between electron orbitals gives rise to an ‘exchange field strength’  $\vec{H}_{\text{exch}}$  which normally tries to align magnetic moments in parallel that are close to one another. Usually, this is the most important contribution to the effective field strength.

The demagnetizing field  $\vec{H}_{\text{demag}}$  is computationally most expensive due to its ‘every individual magnetic moment interacts with every other magnetic moment from the rest of the sample’ nature. This is of the structure:

$$H_{\text{demag},j}(\vec{x}) = \int d^3y G_{jk}(\vec{x}, \vec{y}) M_k(\vec{y}) \quad (5)$$

where the kernel  $G_{jk}(\vec{x}, \vec{y})$  gives the magnetic field at position  $\vec{x}$  produced by a localized Dirac dipole at  $\vec{y}$ .

The effective exchange field strength is phenomenologically modeled by taking the vector (i.e. component-wise) Laplacian of the magnetization:

$$H_{\text{exch},j}(\vec{x}) = c_{\text{exch}} \frac{\partial}{\partial x_k} \frac{\partial}{\partial x_k} M_j(\vec{x}). \quad (6)$$

The magnetocrystalline *anisotropy* term usually is described through a truncated polynomial expansion, which is a *local* function of the magnetization  $\vec{M}(\vec{x})$ , or, in tensor-index notation:

$$H_{\text{anis},j} = \delta E[\vec{M}]/\delta M_j \quad (7)$$

with the energy function being of the form

$$E[\vec{M}] = E^{(0)} + E_j^{(1)} M_j + E_{jk}^{(2)} M_j M_k + E_{jkl}^{(3)} M_j M_k M_l + \dots \quad (8)$$

(Physically speaking,  $E^{(0)}$  is irrelevant and  $E_j^{(1)}$  would behave like another contribution to the externally applied field. Nevertheless, this is the most general form.)

## 2.2 A micromagnetic simulation

Some results of a simple micromagnetic example calculation are shown in figure 3, and have been computed using the script shown in figure 2.

The system simulated is a magnetic disk with a diameter of 150 nanometers (nm) and a thickness of 5 nm. The material parameters are chosen as  $|\vec{M}| = 10^6$  A/m, and  $c_{\text{exch}} = 1.3 \cdot 10^{-11}$  J/m, roughly similar to those of PermAlloy.

The local exchange coupling favors parallel alignment of the magnetization  $\vec{M}$  over short distances, as the black cones representing the direction of magnetization in figure 3 show. This interaction competes with the demagnetization interaction which favors a configuration where magnetic North and South poles connect and which minimizes surface charges. The physical solution for the given geometry and material parameters in the absence of any external magnetic fields is shown in figure 3 (left) and represents a vortex. This closed flux configuration of the magnetization minimizes the demagnetization energy, and incurs only a small energy penalty from the curvature in the magnetization.

Figure 3 (right) shows the resulting equilibrium configuration if an magnetic field of  $H_{\text{ext}} = 40 \cdot 10^3$  A/m is applied, pointing from the left to the right. Comparing the situation without an applied field shown in figure 3 (left) to the situation with the applied field (right), the center of the vortex moves downward. This minimizes the overall energy of the system because a large fraction of the magnetization aligns with the external field.

This is a fairly simple micromagnetic example which should convey the kind of complex physics emerging from competing interactions. Problems like this can often (especially in complicated geometries) only be tackled successfully using numerical simulations.

### 2.3 Multi-physics micromagnetism

The effective field  $\vec{H}_{\text{eff}}(\vec{x}) = \vec{H}_{\text{ext}}(\vec{x}) + \vec{H}_{\text{demag}}(\vec{x}) + \vec{H}_{\text{exch}}(\vec{x}) + \vec{H}_{\text{anis}}(\vec{x})$ , collects the contributions outlined above (which all are of computationally very different type) and make up the conventional micromagnetic model.

There is growing need to include additional physics to these simulations, such as e.g. the extra torque on magnetic moments caused by (spin-polarized) electric current densities. This is required to simulate the effects that may be employed in the data storage and processing devices of the future.

In micromagnetism, most additional contributions to the equation of motion can be expressed through local polynomials in other fields, spatial differential operators of order at most two, and integrals over propagators from long-range interactions. There are reasons based on insights from renormalization theory on the general structure of a hierarchy of short-range corrections to classical field theory that suggest that this is a fairly common situation that should arise in most other phenomenological models of mesoscopic physics as well. Essentially, these concepts are applicable in most applications where the system's free energy functional can be given as a truncated series expansion.

## 3 Multi-physics simulations

The need for and growing importance of multi-physics simulations has been recognized in the computational science and engineering community and industry for some time [10, 11].

Multi-physics simulations are a relatively new computational field in materials science, and often simulations are carried out by using two (or more) simulation codes that simulate one phenomenon each. The different codes are run subsequently and iteratively until a self-consistent solution has been found. However, in general it is desirable to solve all the

equations simultaneously (even though this often means existing codes cannot be used) so that – in particular – time dependent processes can be studied more easily.

Particular sectors of computational engineering have been using multi-physics simulations for a long time, including fluid-structure interactions and aeroelasticity, and combustion chamber simulations.

Commercial packages have become available for mainstream engineering applications [12, 13, 14] but there is still need for tools with either specialized functionality for niche or emerging research domains or capability to exploit particular hardware for high performance computing.

In more detail, commercial multi-physics simulation tools (such as Comsol [13] (formerly FEMLAB), and ANSYS [14]) can perform some of the computations required for micromagnetic simulations (such as computing the current density distribution from a given applied voltage, or computing the diffusion of heat). However, they (at the time of this writing) cannot carry out the complex high-frequency micromagnetic and spintronic dynamics.

While `Nsim` – to the authors’ best knowledge – is presently unique in its combined support for runtime translation of model equations, transparent parallelization, generic tensor-index symbolic notation for physical equations, and end user flexibility through utilization of the capabilities of a well-established scripting language, other frameworks exist that follow an approach towards field theory simulations which has some overlap with `Nsim`’s. These include the commercial packages listed above, Diffpack [15], Fastflo [16], as well as the free systems Elmer [17], FEniCS [18], FreeFem [19], OOMPH-Lib [20], OpenFEM [21], OpenFOAM [22], and the system presented in [23].

## 4 Formal specifications of physical systems

Ideally, automated compilation of field theoretic systems should be able to proceed from a purely formal specification of the equations of motion, the geometry of the system, and the initial and boundary conditions to a working simulation of the time evolution of that system. Work on the `Nsim` prototype system showed major differences in the usability and practicality of different notational conventions. At the time of this writing the symbolic conventions suggested must be considered as still being in a state of flux. We hence report our present findings, warning the reader that these are preliminary and possibly subject to some degree of future change as our understanding of the psychological aspects of mapping physical equations to the ASCII character set increases.

### 4.1 A perspective on abstraction

Considering the history of computer programming, an evolutionary step that has come into reach now is to provide and utilize the linguistic capabilities to directly express field theory concepts and ideas in computer code and leave the details of translating these to (possibly parallel) matrix/vector operations to a compiler. While in the previous visible evolutionary trend towards ever higher forms of abstraction, high hopes and big dreams that ultimately failed to manifest were associated with every step, important progress unquestionably has happened nevertheless. While at no point, we reached the stage that would ‘render debugging unnecessary’, a higher level of abstraction allows one to spend

effort more efficiently on dealing with aspects that are closer to the properties of the part of the real world one tries to model than to the characteristics of the computing machinery on which this model is implemented.

## 4.2 Fundamental concepts

A framework designed for the purpose of simulating multiple interacting physical sectors (e.g. micromagnetism and heat conduction) requires some abstract notions. It should be pointed out that both these concepts *as well as their implementation in the Nsim prototype*<sup>4</sup> are sufficiently general to support physics in arbitrary dimension, rather than just three-dimensional space. We use the following terms:

- A *region* is a (potentially disconnected, potentially multiply connected) subset of the cells of a mesh that describe a material with uniform physical properties. Regions are numbered 1, 2, ... and may have additional *attributes* such as ‘magnetic’ or ‘conducting’ that then can be used when specifying differential operators. As this notion is especially important to define boundary conditions, we extend it to include pseudo-regions associated to non-meshed outer space, which carry negative numbers -1, -2, ... This allows us to use pairs of integers to describe boundaries and designate different types of boundary conditions on different parts of the outer boundary of a material – e.g. Dirichlet (constant potential) boundary conditions on some faces of a conductor and von Neumann (no current flowing off the sample) boundary conditions on others.
- A *site* is a position in the mesh that can carry degrees of freedom. When using first order elements, these are just the vertices of the mesh. When using second order elements, this would also include edge midpoints.
- An *element* is a prescription to associate degrees of freedom to a cell of a mesh (e.g. a magnetization vector and a conductivity scalar). Usually, there will be one element type for every region in the mesh.
- A *degree of freedom* is a single (real floatingpoint) number associated to a site that has a *name* which consists of a string – the *stem* – and an array of integers (possibly of length zero) that describe its *indices*, where index counting starts at zero. The name of the degree of freedom describing the x-directed component of the electrical field strength hence would be  $E[0]$ , while the name of the z-directed flow of x-directed momentum could be named  $J_p[0,2]$ .
- A *field* is a collection of degrees of freedom obtained by associating elements to the cells of a mesh.
- A *subfield* is a subset of the degrees of freedom of a field that share the same name stem. The rationale underlying this concept is that we may have to collect multiple physical fields of different origin and nature into a single entity. For example, in a multi-material micromagnetic simulation, sites belonging to the boundary separating two magnetic materials will have to carry two different types of magnetization.

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<sup>4</sup>With the exception of some surface/surface interaction integrals that use properties specific to three dimensions

- A *primary field* is a field that describes those aspects of the system that can in principle be influenced by the experimenter. In micromagnetism, both magnetization and externally applied field strength are primary fields.
- An *auxiliary field* is an intermediate quantity derived either directly from the primary fields, or from other auxiliary fields. In micromagnetism, the effective magnetic field strength  $\vec{H}_{\text{eff}}$  is an auxiliary field.

### 4.3 The language

The formal specification of a physical system to be simulated consists of:

- A description of the geometry (including information about regions).
- A description of the fields associated to (different regions in) the system.
- The specification of initial and boundary conditions.
- A collection of (local and differential) equations that determine how auxiliary fields are obtained from primary fields.
- (optionally) tweaking parameters for improving the computational efficiency of some particular parts of the simulation.

Considering computer simulations in the broader context of their scientific and industrial environment, there may be important extrinsic aspects associated to some pieces of such a description: In particular, while it may be desirable to be able to define the geometry of some sample through a small number of equations, we can realistically expect that many users will also want to utilize pre-existing geometry descriptions e.g. produced by some mesh generating CAD software. While the `Nsim` prototype includes some basic mesh-generating capabilities to demonstrate the concept of fully equation-based analytic system specifications [24], this so far has not been evolved into a highly efficient mesh generating subsystem. As externally generated meshes can be utilized, work on the geometry specification aspects is presently regarded a lower priority issue.

In the `Nsim` prototype, the layout of a field is specified by providing the association of elements to mesh regions. An element is either a primary element, associating a complete set of tensor degrees of freedom (such as  $E_x, E_y, E_z$ ) to each site in a mesh cell, or is a fusion of other elements. Occasionally, we want to work with a collection of fields of identical layout (i.e. component-wise addition of the entries of the numerical arrays is a sensible operation) in which the degrees of freedom are nevertheless addressed through different names. In the micromagnetic application `Nmag`, this situation occurs e.g. when contributions to the total effective magnetic field strength  $H_{\text{eff}}$  which are of very different physical origin are summed. Experiments with a number of different strategies have shown that a convenient and uniform approach towards such a situation is to introduce ‘derivatives’ of existing field layouts which are produced by renaming the name stems of the degrees of freedom. A code example that demonstrates this technique can be found in appendix A.



### 4.3.1 Differential operators

Differential operators, which get mapped to sparsely occupied matrices acting on the data arrays of fields, are specified as strings that get parsed according to a grammar which is inspired by quantum mechanical bra-ket notation and also supports the Einstein summation convention. In this notation, the Galerkin discretisation of e.g. the heat diffusion operator

$$M_{ij} = - \int_{\mathcal{V}} \frac{\partial}{\partial x^k} \phi_i^{(DT)} \frac{\partial}{\partial x^k} \phi_j^{(T)} d\mathcal{V} \quad (9)$$

is given as:

$$- \langle d/dxk \text{ DT} \mid \mid d/dxk \text{ T} \rangle, \text{ k:3} \quad (10)$$

while the operator computing the divergence of a tensor-valued field of rank two could be specified as:

$$\langle \text{divJ(a)} \mid \mid d/dxb \text{ J(a,b)} \rangle, \text{ b:3} \quad (11)$$

While this ‘core notation’ has been found to be both viable and convenient to use, some of the more complicated extensions are still in a state of flux, especially when involving boundary conditions. We briefly describe each presently supported extension in turn as well as hint at a context in which these become relevant.

#### Surface derivatives

While the `Nsim` prototype at present is based on simplicial (in 3d, tetrahedral) rather than singular homology, i.e. does not allow the association of degrees of freedom to sub-simplices of volume simplices (such as point or line charges), surface derivatives play such an important role for continuity equations that a special notation has been introduced to deal with them. When sparse operator matrices are being computed from abstract operator descriptions by working out integrals over cells of products of shape functions, the field prefix `d/dxj` causes the replacement of the corresponding field basis function by its coordinate derivative. Likewise, the field prefix `D/Dxj` effects the modifications required to produce matrix contributions that correspond to surface divergence jumps for simplex faces across which the field ceases to exist. (The volume integral over the simplex is replaced by surface integrals over the relevant faces, multiplied by the  $j$ -th component of the surface ‘normal’ (rather,  $(d - 1)$ -vector). The translation of expressions in which two surface derivatives occur in the same bra-ket, such as `<D/Dxj phi | | D/Dxj phi>`, causes an error, as such a product of distributions is not well defined mathematically.)

In micromagnetism, these surface derivatives are required to correctly compute the surface divergences of the magnetization field which enter the computation of the demagnetizing field as source terms. (Note that for homogeneously magnetized systems, these surface magnetic charges are the only sources of the demagnetizing field.)

#### Region and boundary restrictions

We may want to restrict some contributions to a differential operator to degrees of freedom associated with some particular mesh regions, or region boundaries. This can be done by adding a restricting qualifier in angle brackets to the name of the degree of freedom. Experience with earlier versions of the `Nsim` prototype has shown that it is surprisingly tricky to define a region specification language that is both conceptually simple and at the same time flexible enough in order to support all the common use cases. The

present version of `Nsim` uses a simple grammar for boolean logic that refers to region properties associated with materials and allows specifications such as `J[not magnetic](2)` or `J[conducting and insulated_boundary](1)`, and could also handle more complicated cases such as `T[(ferroelectric or ferromagnetic) and not boundary]`. While this is not expected to be the final word on region specifications<sup>5</sup>, more simplistic approaches have been shown to be too clumsy in practice.

### Matrix shortening

When employing region-based restrictions, we may want to construct a ‘shortened’ version of some matrix operator which maps (potentially) shortened data vectors to (potentially) shortened data vectors. Shortened vectors only contain the degrees of freedom selected by some particular region restriction and play an important role e.g. when providing boundary values for (say, Dirichlet) boundary conditions, or exchanging data between the FEM and BEM parts of some hybrid FEM/BEM code. The syntax presently used in the `Nsim` prototype is to append a semicolon-separated qualifier to an operator specification that gives the left- and right-hand-side restrictions on the degrees of freedom, as in:

```
<phi || phi>; (L||R)=(*||phi[boundary]).
```

### Residual gauge fixing

When using a linear solvers to invert discretised operators, such as when solving a Laplace equation to obtain a potential from a charge density, we will have to address the ‘residual gauge symmetry’ that corresponds to a (spatially constant) shift of the potential  $\Delta\psi = \Delta(\psi + c)$  which reduces the rank of the Laplace operator’s matrix by one for every component of connection. Linear algebra libraries usually provide functions to deal with such situations<sup>6</sup> and generally should be preferred over other solutions (such as introducing local modifications to the matrices), as other approaches may cause a noticeable slowdown due to unnecessary communication overhead in parallel computations. At the time of this writing, information about such null spaces has to be specified in `Nsim` when setting up a linear solver to invert a differential operator. In earlier versions, this was provided as a grammar extension to the operator specification itself. It is not yet entirely clear what the best approach is here.

### Dirichlet boundary conditions

When working with Dirichlet Boundary Conditions, we may want to exclude certain rows and columns from the matrix but introduce ones on the diagonal in order to maintain regularity. This at present can be specified using semicolon-separated modifiers of the form `LEFT=RIGHT`, as in:

```
<d/dxk phi[vol] || d/dxk phi[vol]>; phi[boundary]=phi[boundary], k:3,
```

but again, this notation is considered to be preliminary and somewhat unsatisfactory.

### Periodic boundary conditions

There are a number of subtle aspects associated to periodic boundary conditions which are explained in detail in [25]. Essentially, periodicity is specified by associating the

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<sup>5</sup>especially in conjunction with code-generated equations where an infix notation of logic operations may not be the most natural and convenient representation

<sup>6</sup>such as the `MatSetNullspace` function in the PETSc [1] library employed by `Nsim`

mesh with information about sites that are to be identified (which need not be at outer boundaries). Linear operators discretized on such meshes usually will want to respect periodicity. In `Nsim`, degrees of freedom subject to periodic identification occur multiple times in field data vectors, as this greatly simplifies some operations, such as interpolating field values over the mesh. Duplication of degrees of freedom must not occur, however, in the state vectors on which the time integrator acts, as this would cause serious problems with stiff solvers. Therefore, `Nsim`'s support for periodic boundary conditions requires mapping data vectors back and forth between 'long' representations with duplicate entries and 'short' representations without, as well as special tricks when automatically generating a Jacobi matrix that acts on 'short' vectors but may involve (in its definition) differential operators that deal with 'long' vectors.

As a consequence of this approach, operators at present have to use a periodicity modifier, as in `<phi||phi>; periodic=phi`. The effect is that matrix contributions computed for one instance of a degree of freedom subject to periodic identification will be added for other copies as well.

### Generalized second order operators

Generalized forms of Laplace's operator play an important role in many systems. One prominent example is the computation of the electric potential from fixed surface potentials when conductivity is a function of space (or indeed even a dynamic field). Here, we have

$$\vec{j} = \sigma E, \quad E = -\vec{\nabla}\Phi, \quad \vec{\nabla} \cdot \vec{j} = 0, \quad (12)$$

hence we usually want to solve an equation of the form

$$\vec{\nabla} \left( \sigma \vec{\nabla} \Phi \right) = 0 \quad (13)$$

with given boundary conditions. In a numerical discretisation, there is a subtle difference between applying two first-order operators in succession, and applying one second-order operator instead that captures the same physical idea: This is easily seen by observing that the split operator approach would produce next-to-next-neighbor contributions where the single operator approach would only have next-neighbor contributions.

The syntax used in `Nsim` to specify operator matrices that depend on such 'middle fields' is `<d/dxk rho|sigma|d/dxk phi>,k:3`. In the version of `Nsim` published at the time of this writing, a working implementation of code for populating and recomputing sparse operator matrices that involve middle fields is present, but this functionality is not yet accessible from the user level.

### 4.3.2 Local non-linear equations

Apart from auxiliary fields that are computed by applying differential operators to more fundamental fields, and hence 'peek' the physics in the neighborhood of a given site, there also are fields which are being obtained directly from information given at the site in question: These fields are usually called 'algebraic'. In micromagnetism, we encounter both situations in different contributions to the effective total field strength `H_total`: The exchange field strength is obtained by applying a differential operator to the magnetization field that measures how much it 'bends' in the neighborhood of a given point, while the anisotropy field strength is a (potentially complicated) polynomial in the local components of the magnetization vector only.

Any formalism devised to express the computation of auxiliary fields from other fields residing at the same site imposes a restriction on the versatility of the framework unless it is computationally complete. Hence, the `Nsim` prototype provides both a convenient tensor-index formula notation for local operators as well as a way to by-pass it and directly provide a piece of C code that can implement arbitrarily complicated local transformations on fields. Internally, the tensor notation mechanism sits on top of the more flexible mechanism that allows providing C code and uses both a term parser and C code generator. In both cases, the C code that implements local operations utilizes a number of machine-generated macros that check the presence of particular subfields at a given site and allow access to their contents.

The problem with user-provided C code is that it presently cannot be derived symbolically to auto-generate entries in the Jacobi matrix required by the ODE solver for time evolution, so systems that feature both local equations not expressible in the present grammar and stiff behaviour that requires obtaining a good approximation to the Jacobi matrix are not well supported yet. The general expectation is that in such situations, one can either afford the extra effort required by the time integrator library to internally generate an approximation to the Jacobian, or ask for an extension of the `Nsim` prototype to provide additional expressive power to the grammar of local operations: The `Nsim` developers would like to hear from users who run into such problems.

The formula notation based specification of a local operation must provide the ranges of silent indices, a listing of auxiliary local buffers to be used intermediately in the computation, and a sequence of assignments whose left hand side is a subfield degree of freedom and whose right hand side is a tensor polynomial. This tensor polynomial may involve pre-defined constant tensors such as the  $\epsilon_{ijk}$ , which is used to express vector cross products. The Landau Lifshitz and Gilbert equation of micromagnetism (1) can be expressed in this notation as:

```
%range i:3, j:3, k:3, p:3, q:3;

dmdt(i) <-  C1 * eps(i,j,k) * m(j) * H_eff(k)
            +C2 * eps(i,j,k) * m(j) * eps(k,p,q) * m(p) * H_eff(q)
            +C3 * (1.0 + (-1.0)*m(j)*m(j)) * m(i)
```

## 4.4 Field dependencies

Auxiliary fields are computed – sometimes via complicated dependency hierarchies – from the primary fields. Internal consistency in a simulation framework demands that the manipulation of a primary field followed by reading off the value of an auxiliary field which depends on this primary field (directly or through intermediate quantities) automatically triggers the recomputations necessary to provide the updated value: the user of a simulation framework expects to see a consistent picture where values of auxiliary quantities always are automatically up to date. This is an important semantic aspect in addition to the syntactic rules for defining systems. For micromagnetism, the dependency tree of primary and auxiliary fields is shown in figure 4 (ignoring dependencies between vectors distributed across all computational nodes and sequential copies on the master node).

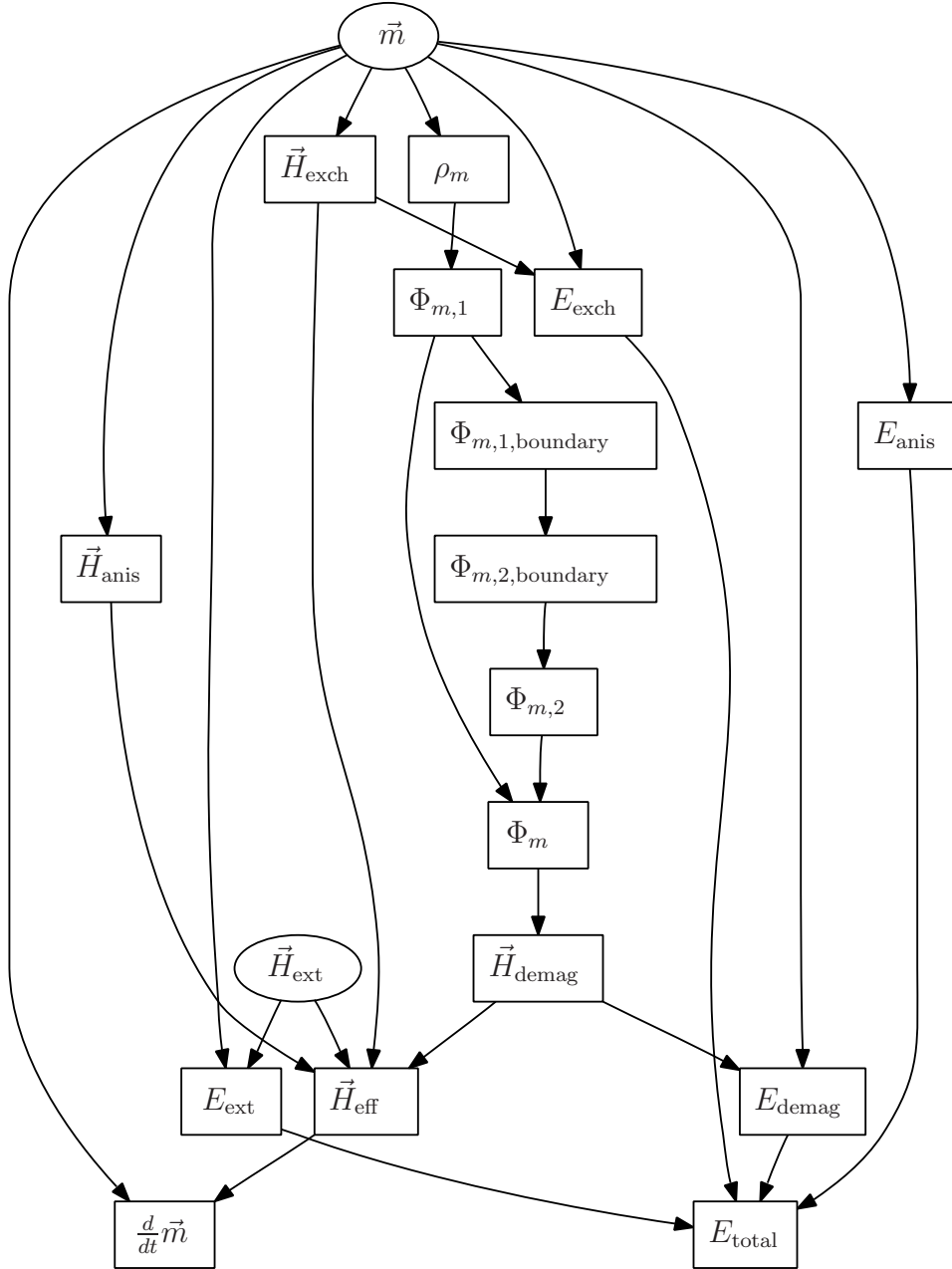


Figure 4: Primary and auxiliary fields in micromagnetism (simplified).

## 4.5 Other examples

Due to the large number of different relevant physical effects – some of them computationally demanding – micromagnetism is a particularly heavyweight application of the `Nsim` compiler prototype. Simpler physical models to which the `Nsim` framework should be even more readily applicable include:

- Heat-flow and thermalization problems.
- Combined electric/heat conduction problems.
- Landau-Devonshire type models of ferroelectric materials.
- Ginzburg-Landau theory of superconductors.
- Turing’s reaction-diffusion model of morphogenesis for pattern formation on animal skins.

A fully worked out example for the last item is given in appendix A.

## 4.6 Physics beyond this language

While the framework described here is sufficiently general to deal with a quite broad class of problems in classical field theory, there are a number of conceptual limitations. The presumably most relevant ones are:

- It presently cannot handle problems that involve hyperbolic equations that require a Riemann solver, i.e. hydrodynamic problems.
- The abstract framework does not yet provide approaches to couple field theory to non-field-theory physics (e.g. field-particle interactions as required to model particle detectors, or coupling to small-scale molecular dynamics models as used e.g. to study crack formation).
- The framework also does not yet support specifications of dynamic (moving) boundaries.
- Theories that require numerical models involving higher derivatives (such as the bi-harmonic equation in elastomechanics) cannot yet be expressed in the abstract operator language.

While these limitations can be overcome, they are beyond the scope of this work.

# 5 The `Nsim` compiler prototype

Some of the technical aspects underlying the `Nsim` compiler – especially those related to parallel computing – warrant a more detailed discussion. Again, we will frequently refer back to the `Nmag` micromagnetic library whenever there is need an example to explain some particular technique.



## 5.1 Bookkeeping over field degrees of freedom

A central data structure in the `Nsim` compiler is the *field layout description*<sup>7</sup>. The role of this field layout description is to provide information on how to physically interpret the data contained in a numerical vector that describes the state of a discretised field.

In the current implementation of `Nsim`, the field layout data structure is constructed from a geometrical specification of the mesh and additional information on the association of (abstractly described) elements to mesh cells as a function of the cell’s associated region number. It would be rather straightforward to extend `Nsim` in such a way that it also can handle other types of field discretisations that are based on more specialized meshes (such as regular grids), but this has not been implemented so far.

At present, the meshes are taken to be composed of simplicial cells of arbitrary(!) dimension (i.e. tetrahedra in three dimensions, pentatopes in four). An abstract element, which is associated to the cells of the mesh by region, provides information about the degrees of freedom belonging to this cell (and usually shared with neighboring cells). An element may introduce multiple physical degrees of freedom, and even multiple *types* of degrees of freedom at the same time (e.g. three components of the electrical field strength, three components of the magnetic field strength, and a mass and charge density to describe the state of a plasma.) The actual location of a degree of freedom may be given as a weighted average of the simplex vertex coordinates (for higher order elements), and the corresponding shape functions are given as polynomials in barycentric coordinates.

The individual physical degrees of freedom are taken to be real-valued only. While it occasionally would be useful to support complex-valued quantities as well, this runs into problems with `Nsim`, as the underlying sparse matrix linear algebra library (PETSc) cannot handle both real and complex linear algebra at the same time within a single program. This, however, is a purely technological rather than a conceptual limitation. While a generalized multiphysics framework certainly has to support scalar and vector degrees of freedom, it should also provide higher order tensors of arbitrary rank to model quantities such as stress, or flow of angular momentum (as e.g. associated to spin-polarized currents). Furthermore, fields may have internal degrees of freedom, i.e. some of the indices of a multi-indexed quantity may not correspond to spatial directions. While this situation is very common in non-abelian gauge theories (such as quantum chromodynamics where QCD ‘photons’ come in eight different varieties), there are few (if any) well known examples in condensed matter physics. This generalization nevertheless is so straightforward that there would be no point in not supporting it as well, however.

The field layout data structure has the capability to provide information about the type and indices of a degree of freedom as well as its physical location in space (both in real coordinates as well as in the form of a weighted average of the positions of mesh vertices), its association to mesh cells and the corresponding shape functions, the total volume associated to the ‘tent’ spawned by the shape functions, other degrees of freedom residing at the same site and similar bookkeeping information.

The most important operations that use field layout information are:

- Extracting a particular subfield from the numerical data describing a multi-subfield field. This situation can arise when part of the full configuration vector of all degrees

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<sup>7</sup>For historical reasons and due to `Nsim`’s FEM background, this is called a ‘*mesh with elements (mwe)*’ in the code.

of freedom (which e.g. is handled by the time integrator) has to be split and passed on to individually developed parts of the simulation that deal with specific physical sectors (such as e.g. heat diffusion).

- Re-Uniting subfields into a unified field vector (the opposite operation of the previous one).
- Extracting some degrees of freedom of a given subfield into a shorter vector containing only a selection of sites (e.g. some particular surface).
- Inserting data from a restricted vector into a longer vector (the opposite operation of the previous one).
- Setting up bookkeeping information for calling machine code which was generated to handle non-linear purely local ‘reaction-type’ equations later on. (I.e. assembling tables of pointers into multiple fields, one for every site, so that compiled code can access these tables to find and identify the numerical values of individual degrees of freedom living at the given site.)
- Probing the value of a field at an arbitrary position, using the analytic shape functions and interpolation.

Frequently, one wants to use field vectors which use different names for individual subfields, but nevertheless are structurally compatible, i.e. component-wise addition of data vectors is a sensible operation. The most immediate example of such a situation is the handling of an equation of the type:

$$M(j) = M(j) + dt * dM_{dt}(j) \tag{14}$$

As was mentioned in section 4.3, usability experiments have shown that a useful approach to handle this situation is to implement *aliasing*: the `Nsim` user interface provides a function (presently named `mwe_sibling()`) that is given a field layout as well as subfield name substitutions and produces another ‘sibling field layout’ which is compatible with the original one (in the above sense) but uses a different set of names for subfields. This can be implemented very efficiently if care is taken that the degree of freedom (dof) data structure does not contain a reference to the subfield name but we instead use a separate function which maps a dof plus a field layout data structure to a subfield name. Then, virtually all of the entries of the field layout data structure (with the exception of the vector containing the abstract elements associated to mesh cells) can be shared between the original and the aliased field layout, making aliasing very cheap in terms of memory requirements. Furthermore, there are some slightly expensive entries in the field layout data structure which are computed on demand when first needed, such as information about all neighboring sites that carry a given subfield. (This is useful e.g. in micromagnetism to find out whether the magnetization vector changes so much between adjacent sites that simulation results cannot be trusted.) These can be shared in such a way (by introducing an extra indirection level) that computing this information for one field layout from a set related through aliasing will also make this information available for all others at the same time.

The present `Nmag` prototype discerns between primary and sibling field layouts and does not allow secondary aliasing of aliased fields in order to limit complexity. (This artificial restriction could be removed.)

An important issue with fields is that a sparse matrix produced from an operator via Galerkin discretisation does *not* represent the linear mapping from discretized field vectors to discretized field vectors corresponding to the original operator. This can easily be seen by convincing oneself that the sparse matrix  $I$  corresponding to the identity operator is the matrix of integrals over products of shape functions. In some situations, this is just what is required. In others, we have to go from a vector of coefficients in dual space back to a vector of coefficients of basis functions. In what follows, we will refer to dual space data vectors as ‘discretised co-fields’. In some situations, these play an important role as they encode information about spatial integrals, e.g. when integrating total outflux of a current across a surface. In others, we have to go from co-fields to fields. While there is only one mapping that is compatible with the natural mapping from fields to co-fields given by the identity operator (i.e. solving the corresponding linear equation system), this occasionally is not helpful, in particular as it destroys locality properties: Considering the combined two-step process of applying a matrix and solving an equation system, we effectively work with a nonsparse linear mapping. If this contributes to the Jacobian of the equations of motion, this matrix will correspondingly become nonsparse and difficult to handle. For this and other reasons, we usually go from co-fields to fields by dividing every vector entry by the integral over the shape function associated to the corresponding degree of freedom (cf. [26]).

During the development of the `Nsim` prototype, the strong distinction between field and co-field data vectors that was implemented by making use of the OCaml type system gradually turned out to be more a hindrance than an advantage, suggesting that soft flagging of numerical data as representing a field or a co-field may be more appropriate.

## 5.2 Dealing with field dependencies: the inference mechanism

Auxiliary quantities are computed from the dynamical degrees of freedom via either purely local (potentially nonlinear) operations, or the application (or inverse application, such as in solving a Laplace equation) of differential operators.

More complicated auxiliary fields that involve both differential and non-linear operations usually can be regarded as being defined in terms of a sequence of intermediate auxiliary quantities where each step in the sequence only involves one of these two types of operations. In effect, this means that there is a dependency tree for auxiliary fields which is rooted in the primary fields. For the micromagnetic model, this tree is shown in figure 4.

Auxiliary fields have to be updated in two different situations: either as part of the effort to compute the new velocity vector  $\dot{y}(t)$  from the configuration vector  $y(t)$  when performing time integration or to reestablish consistency whenever the user changed the physical configuration and reads out some auxiliary quantity from the system. The control logic required to keep track of the necessary updates of derived entities mandated by changes to source entities basically is the same that also underlies the ‘make’ utility program which deals with dependencies of source and derived files belonging to a software project.

While `Nsim` provides such an inference engine which will keep track of auxiliary fields

that have become invalid, the present prototype requires this dependency tree to be explicitly specified by the user. As this information can be derived mechanically from the user-provided definitions of the auxiliary quantities, it would be both feasible and highly desirable to extend the compiler in such a way that the dependency tree can be generated automatically in such a way.

In addition to the forementioned purely semantic aspects, the dependency inference engine also handles buffer updates required to transport numerical field data between individual processes in a parallel computation: Multiple manipulations of primary fields will not trigger parallel communication unless some parallel computation is executed that uses these fields.

### 5.3 Compiling differential operators

In the `Nsim` prototype, the translation of a differential operator to a sparse matrix is a three-stage process. In the first stage, the operator string is parsed. (The corresponding parser being generated from a grammar file by a conventional LALR(1) parser generator.) In the second stage, the left hand side and right hand side field layouts are analyzed for all relevant element combinations and a corresponding internal table is constructed which contains functions that add contributions to the sparse operator matrix if given the simplex to act on. Both these steps are fast and performed only once. The resulting table of functions is then used in a third stage to initialize the sparse operator matrix, and can be re-used to re-initialize the matrix multiple times (e.g. when a ‘middle field’ changes, or nodes are moved in space). In a parallel computation, the internal function table is generated centrally and broadcast over all nodes for subsequent distributed matrix initialization. This is greatly facilitated by building the compiler on top of an infrastructure that supports the serialization of functions (rather, closures) into a network-transportable representation.

Internally, the various amendments that can be made to an operator specification correspond to small modifications on the functions that actually generate matrix entries. As the matrix populating function resulting from stage 2 is fully polymorphic with respect to the few matrix operations required (i.e. adding an entry, flushing, making a matrix, finishing setup), higher-order programming trivializes most of these modifications. E.g. periodic boundary conditions are implemented by wrapping up the function making a matrix entry in such a way that multiple entries are being made for degrees of freedom that have multiple images on the mesh.

When the matrix-population functions are used to populate PETSc matrices for the first time, some issues arise in conjunction with pre-allocation techniques: The present version of PETSc does not release memory that was pre-allocated when creating a sparse matrix, and as `Nsim` at present does not pre-compute the number of entries in each matrix row, so a trick is employed in order to release unused memory which consists of copying the finished matrix and freeing the original<sup>8</sup>.

The compilation of differential operators is the most complex piece of code within the `Nsim` codebase that lies at the core of the system, with other parts having evolved around it.

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<sup>8</sup>The authors thank the PETSc developers for telling them about this.

## 5.4 Solving operator equations

Whenever a physical system involves very fast processes that come to an equilibrium on time scales much shorter than those of interest, we may benefit from employing potential theory to find those equilibria that both depend on and influence the slower physics. In micromagnetism, this certainly is the case for the electromagnetic field: a change in magnetization at one end of a sample of size  $\ell = 1\ \mu\text{m}$  will take a characteristic time of about  $\ell/c \approx 3 \cdot 10^{-15}\ \text{s}$  to travel to the other end, while characteristic time scales for magnetization dynamics are in the range of  $10^{-12}\ \text{s}$ . Hence, ignoring retardation and radiative effects is a good approximation in the computation of the magnetic self-interaction of the sample. The situation in micromagnetism is considered to represent a generic case: the computation of some auxiliary field (the demagnetization field strength  $\vec{H}_{\text{demag}}$ ) often involves a number of intermediate steps, some of them requiring to solve a potential equation. In micromagnetism, the problem of finding  $\vec{H}_{\text{demag}}$  corresponds to removing the longitudinal modes of  $\vec{M}$ , as  $\vec{B} = \vec{H} + 4\pi\vec{M}$  and  $\vec{\nabla} \cdot \vec{B} = 0$ . This can be achieved either via Fourier transformation on a regular lattice<sup>9</sup>, or in the the Finite-Element/Boundary-Element Method approach via a more involved computation where two Laplace equations have to be solved for one computation of  $\vec{H}_{\text{demag}}$ : One to find the magnetic scalar potential corresponding to  $\vec{\nabla} \cdot \vec{M}$  with natural boundary conditions, and one to extend the boundary corrections that give ‘Dirichlet boundary conditions with zero potential at infinity’ from the surface to the interior.

While there are many problems where just a single Laplace equation has to be solved (e.g. to get the electric current distribution in a conductor), more involved situations similar to the one described above are assumed to be somewhat common. At present, `Nsim` supports these by allowing the user to define linear solvers on top of operators and then specify (parallelizable) sequences of linear algebra operations that may involve applying a solver, going from a co-field to a field, etc. While the underlying technology has been implemented and can be employed to define even complicated calculations, the problem of introducing a convincingly convenient notation has not been addressed yet. The developers’ present view is that supporting a terse notation for two or three very common cases that include obtaining a potential from a charge distribution as well as removing some longitudinal part of a tensor field most likely covers a large part of all relevant applications. The ability to specify computation sequences in detail should be retained for unusual situations.

## 5.5 Nonsparse linear operators

While every differential operator will produce a sparse matrix when discretised in the straightforward way on a cell structure in space as a consequence of its localization properties, there also are situations when long-range effects which couple degrees of freedom at arbitrary positions have to be modeled. Whenever this happens, the system often becomes very challenging to simulate, doubly so in the particular example of micromagnetism as in addition to long range interactions, stiffness of the system becomes an issue as well.

From the physical perspective, long-range interactions are closely related to very light

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<sup>9</sup>The OOMMF [27] package is based on such an approach.

bosonic exchange particles, with the most prominent and therefore dominant case being that of a massless vector boson such as the photon. Hence, those problems that require the inclusion of long range interactions very frequently can be tackled by employing potential theory in some clever way, with the standard problem being the solution of Poisson’s equation with Dirichlet boundary conditions at infinity. This can be regarded as a third class of boundary conditions of great practical importance in addition to the more straightforwardly defined Dirichlet and von Neumann boundary conditions. On unstructured meshes, a widely used technique to solve this class of problems was given by Fredkin and Koehler in [28]. Essentially, their hybrid Finite Element/Boundary Element method boils down to the introduction of a square  $N \times N$  matrix,  $N$  being the number of boundary degrees of freedom, that encodes all the information about boundary-boundary interactions. For potential problems using first order elements, an analytical formula given by Lindholm [29] that describes the potential of a triangular dipole layer with linearly varying source density can be used to compute the matrix elements. While this technique works sufficiently well to be employed e.g. in micromagnetism, there are a number of problems:

- Even for moderately sized simulations, the boundary element matrix may require a considerable amount of memory, as well as setup time. (10 000 surface nodes would require  $\sim 800$  MB of RAM using standard 64-bit floatingpoint element representations). This is especially a problem with thin film geometries.
- Lindholm’s formula suffers from numerical cancellation problems in some geometric configurations.

In a FE/BE implementation, the latter problem may be alleviated to some degree by internally using extended floatingpoint numbers for the computation, but this often is impractical. A numerically more useful equivalent of the original formula hence would be desirable. Concerning the former issue, there are approximation techniques to reduce memory footprint such as using hierarchical matrices which are based on a clustered approximation of propagators  $G(x - y) \sim \sum_k c_k G(x) \cdot G(y)$  [30]. The `Nsim` prototype supports explicit computation of a nonsparse  $N \times N$  boundary element matrix for first order elements based on Lindholm’s formula and also can utilize the `HLib` [31] library to use matrix compression<sup>10</sup>. Support for quasi-long range interactions, i.e. forces mediated by particles whose mass corresponds to a length scale somewhere between the cell and the mesh size is not implemented at present.

## 5.6 Periodic boundary conditions

The term ‘periodic boundary conditions’ is used for two conceptually different ideas: on the one hand to reduce the finite-size artefacts in computer simulations of the statistical properties of a sample, and on the other hand to simulate some of the relevant processes associated to a single cell in a repetitive sample. Subtle issues arise when systems made up of very many periodic copies of a fundamental unit are to be simulated employing periodic boundary conditions while they also feature long range interactions. In such a situation, it usually becomes necessary to amend the numerical model with relations between the wave-vector-zero components of fields. Again, this situation is easy to understand through the

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<sup>10</sup>Due to license issues, `HLib` does not come with `Nsim`, but has to be obtained and installed separately.



example of micromagnetism: While it may be possible to learn a lot about the behaviour of a system made up of 1 000 000 identical cells by simulating a single cell in the interior with periodic boundary conditions, the relation between the average of the magnetization  $\langle \vec{M} \rangle$  and the average of the demagnetizing field  $\langle \vec{H}_{\text{demag}} \rangle$  over the cell are still determined by the shape of the (faraway) boundaries of the sample only. There is some initial support for these ‘macro-geometry’ effects in `Nsim`, as they are relevant for micromagnetism [25], but it is not yet entirely clear whether this is sufficiently generic for other applications where such situations arise.

Subtle long-range issues aside such as those described above, periodic boundary conditions are supported by allowing meshes to be associated with information on the identification of vertices, from which identifications of sites also follow (which is especially relevant for higher-order elements). A generalization that would often be useful but is not yet supported would be to allow arbitrary affine-linear transformations between the fields living at different periodic copies of a site. This would e.g. allow to simulate systems with axial symmetry by imposing suitable ‘periodic boundary conditions’ on a wedge, or to set up systems in which potentials on opposite faces are identified up to a constant, etc. This approach would, however, raise a number of somewhat tricky technical issues related to the automatic generation of Jacobi matrices.

## 5.7 Local non-linear equations

The other elementary building block of field operations (apart from linear, differential field operators) is arbitrary (i.e. usually non-linear) *site-local* manipulations of fields. In combination, and through the introduction of intermediate auxiliary fields (such as e.g.  $H_{\text{eff}}$  in micromagnetism), these basic operations cover the vast majority of field operations encountered in applications.

The notion of *site-local* operations encompasses all manipulations on a set of fields which are to be performed at every mesh site in the same way, and operate on the subfield components of these fields which are located at the specific site only. This basically corresponds to ‘considering position dependency as implicitly being understood’ in physical notation when giving an equation such as the Landau-Lifshitz and Gilbert equation in the form (2).

We may want to use site-local manipulations that involve highly unusual operations which cannot be expressed easily in arithmetic notation. (For example, we may want to use different manipulations depending on whether some temperature is above or below a critical value.) As a consequence, maximum flexibility demands the capability to allow arbitrary user-specified code to specify local physics. This code nevertheless has to be executed fast, therefore the `Nsim` prototype compiler resorts to employing runtime compilation techniques, as explained in section 5.11.4.

Before sending user-supplied code to the C compiler, `Nsim` wraps it up in a block if `#define/#undef` macros which allow the user code to refer to local subfield components directly by their name and indices, regardless of the field data vector they are located in<sup>11</sup>. Also, `Nsim` provides C macros with which presence of a particular subfield at a given site may be tested, as this may depend on the site in heterostructures.

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<sup>11</sup>The observed utility of this approach was the underlying reason for implementing ‘field aliasing’, cf. section 5.1

From the perspective of user-supplied local code, the `Nsim` framework provides a context in which to execute this code over all sites of a mesh on a number of fields (and co-fields) via wrapping definitions, as well as behind-the-scenes bookkeeping over site-dependent offsets into the field data vectors, plus automatic compilation-on-demand.

While it is crucial to provide maximal flexibility to the user through the option to specify arbitrary code for site-wise execution, it is just as important to also provide an alternative interface which, rather than asking the user to write C code, allows specification of equations in algebraic notation. This is achieved by employing a LALR(1) parser generated by OCaml’s equivalent of ‘yacc’ from a formal grammar specification and translating algebraic notation to C code internally, which then is provided to the general mechanism. Also, algebraic notation allows auto-generation of derivatives of equations of motion (through some internal symbolic algebra) as needed for the Jacobian which should be known (at least approximatively) to successfully employ some time integrators, such as CVODE. (Cf. sections 5.8 and 5.10.)

## 5.8 Computation of the Jacobian $dy_j(t)/dy_k$

A not too uncommon situation is that the physical system under investigation may be numerically challenging due to its stiffness. In micromagnetism, this happens due to a gap of more than two orders of magnitude between the characteristic time scales of the reaction of the system to a strongly localized perturbation. This comes from different physical effects (in the simplest case, the long-range demagnetization field and the extremely strong effective exchange coupling that tries to make closely spaced magnetic degrees of freedom align and move in unison). There are a number of code bases that implement time integration algorithms for stiff systems which often can be used in a ‘black box’ fashion. Normally, the user of such a time integration library has to provide both a function that computes the velocities, given some particular state of the system, as well as a function that computes the Jacobian. Roughly speaking, the Jacobian helps to find a transformation from the fundamental degrees of freedom to a more useful basis which allows to separate fast processes (‘high frequency ringing’ of the system) which often are not excited in physical systems from the more interesting collective slow dynamics.

The Jacobian usually is a function of the configuration and time, and as it is expected to be costly to compute, the time integration library will try to avoid recomputation of the Jacobi matrix as much as possible. (Evidently, some heuristics has to be used here, as it cannot be known beforehand how many processor cycles the computation of the Jacobi matrix will take in a particular situation.)

In principle, the Jacobi matrix can be computed automatically when given the equations of motion. In reality, most physical simulations use hand-written low-level code (usually C or FORTRAN) to implement the computation of the numerical matrix entries. For systems with more complicated equations of motion (such as micromagnetism), the implementation of the code that computes the Jacobian can become a rather tedious and frustrating process that is prone to errors which here unfortunately are easy to make but fiendishly difficult to track down.

For this particular reason, `Nsim` provides capabilities to automatically generate the Jacobian from the symbolically specified equations of motion. While it would in principle be possible to just use these as they are and symbolically take second derivatives, one discovers in practice that it makes sense to introduce some additional flexibility in the

specification of the Jacobian. One important issue is that one may use equations of motion for the Jacobian (which only needs to be approximatively right) which are slightly different from the system’s actual equations of motion. For example, if extra nonphysical terms have been introduced for the sole purpose of numerical stabilization, one will usually want to simplify the Jacobian by not including these. A second type of important simplification that must be supported is to allow the use of approximations to derivatives of dependent fields. In the particular case of micromagnetism, it is useful to approximate  $\delta H_{\text{eff}}/\delta M$  by  $\delta H_{\text{exch}}/\delta M + \delta H_{\text{anis}}/\delta M$ , omitting the contribution from the demagnetizing field (which would at the same time be very costly to compute, not expressible through a sparse matrix contribution to the Jacobian, and not a source of fast dynamics).

The present internal design of the component providing symbolic auto-generation of the Jacobian in the `Nsim` prototype presumably has not settled down to its final form yet, as it still appears to be somewhat unwieldy in some situations. At present, the interface works in such a way that the user specifies both an equation of motion, such as e.g. a string representation of the Landau Lifshitz and Gilbert equation, as well as additional information on contributions to the derivatives (with respect to the configuration degrees of freedom) of the fields that appear in the equation of motion. This is given as a list, one entry for each field that enters the equations of motion (with meaningless entries such as  $\delta \vec{M}/\delta \vec{M}$  ignored). Each list entry itself is a list of contributions which will be summed and either provide a local non-linear (at present, only polynomial) equation, or a name of a sparse operator. The former case is used for providing the contribution to  $\delta H_{\text{eff}}/\delta M$  that comes from the anisotropy field strength  $\delta H_{\text{anis}}/\delta M$ , while the latter is used to for providing the  $\delta H_{\text{exch}}/\delta M$  contribution.

The system then internally ‘precompiles’ this information to a function that can be called in order to (re-)populate the Jacobi matrix. In a parallel computation, this is handled as with other sparse matrices: the population function is generated centrally and then distributed over the cluster. Evidently, such a matrix population operation also requires making the data necessary to work out the individual contributions to all nodes (i.e. a MPI `allgather()` operation on relevant fields). Some complications arise as recomputation of the Jacobian is triggered by the time integrator: on the one hand, rather than just updating the Jacobian  $J$ , the sparse matrix  $\mathcal{K} - \gamma J$  (with  $\gamma \in [0, 1)$  given) has to be created and updated (in parallel) as well. Furthermore, when doing simulations with periodic boundary conditions, the situation is complicated by the necessity not to duplicate entries in the state vector of the time integration library used by `Nsim` on the one hand and the desire to directly use sparse matrices which use duplicate entries on the other hand. Hence, the function that is triggered internally to recompute the Jacobian has to do some automatic index mapping to hide this mismatch.

An earlier approach used in `Nsim` to compute the Jacobi matrix  $J$  involved the pre-computation and distribution of a data structure that provided a symbolic polynomial for the computation of each nonzero matrix entry. This was soon abolished as it turned out to use prohibitive amounts of memory.

## 5.9 The ‘physics engine’ abstraction

When setting up a simulation, `Nsim` translates a complete specification of all field layouts, fields, sparse and nonsparse operators and linear solvers, as well as local equations and field dependencies to an object-like data structure that provides methods to set and read

off fields, and to advance time<sup>12</sup>. While this ‘monolithic’ approach greatly simplifies the compiler, it ultimately should be broken up so that it becomes possible to freely add (and remove) operators to a simulation object after initial setup. Technically, this would be possible with rather little effort in the present `Nsim` codebase, as most of the internal bookkeeping of dependencies of data structures on one another are compatible with such a restructuring.

## 5.10 Parallelized time integration

While the idea may be seductive to simplify the code structure of a parallel multiphysics simulation framework by employing parallel computing only for computationally expensive linear algebra (e.g. solving linear equations) and keeping time integration centralized in the controlling process, one finds that for challenging problems that involve stiff dynamics (such as micromagnetism), such an architectural design becomes a major bottleneck: Measurements show that about as much numerical effort is required to deal with stiffness in the time integrator as is needed to compute all the expensive auxiliary fields. Hence, time integration has to be fully parallelized as well.

In some situations, time integration has to respect additional constraints which must not be violated by numerical drift. Such a situation occurs in `Nmag` with the magnitude of magnetization and is dealt with by introducing an additional term in the equations of motion for numerical stabilization, as explained in section 2.1.

The `Nsim` prototype presently utilizes the readily parallelizable CVODE time integrator from the Sundials [3] library. As this is an adaptive algorithm whose implementation in the Sundials library experiences problems with fixing step sizes, the `Nmag` application also contains a fixed-step Heun integrator for applications where this is required. The incentive to include this alternative comes from the desire to simulate thermal fluctuations based on Langevin dynamics. However, as the duplication of degrees of freedom due to periodic boundary conditions needs special handling in time integration, this alternative integrator does not yet support periodic boundary conditions.

## 5.11 User interaction

The idea of using computer simulations to study some particular aspect of the behaviour of a physical system intrinsically calls for a certain level of flexibility. One rather obvious reason is that one would like to be able to automatize the processing of simulation results to tables, diagrams, and other images. In addition to this, there are situations where one would like to use a bit of automatized choreography for performing a parametrized sequence of simulation runs (‘computational steering’). A prime example for this would be to run a series of individual micromagnetic simulations where the externally applied magnetic field strength varies in a controlled way in order to produce some particular switching sequence. Here, one would ideally want to be able to wrap some control and post-processing code around the simulation core in such a way that the mapping of a given switching sequence to a number of diagrams which describe the physics of the process is fully automatized.

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<sup>12</sup>In the present version of the `Nsim` prototype, this is (for historic reasons) named a ‘linear algebra machine’

### 5.11.1 Standalone programs vs. libraries

While such situations that basically ask for a Turing-complete level of flexibility are rather widespread, many specialized software packages have been written where the a design mistake has been made to initially underestimate the amount of flexibility that eventually would be required and trying to mend this progressively in incremental steps. Typically, such systems gradually evolve from being able to read very primitively structured configuration files towards using a LALR(1) parser in order to deal with more complex configuration files towards supporting some rudimentary form of variables, arithmetics, and control structure. Subsequently, a need arises for container data types such as arrays (which also introduces a number of tricky memory management issues), then file I/O, and finally the capability to interface C libraries and a debugger.<sup>13</sup>

A reasonable approach to avoid this problem is to provide maximum flexibility from the beginning through designing the system in such a way that it provides all of its special capabilities in the form of a software library and interface this to some existing popular programming language with a large user base.

### 5.11.2 The Python scripting language as an especially attractive option

For `Nsim`, the design decision to utilize Guido van Rossum's 'Python' scripting language [5] (and hence give `Nsim` the form of a Python library) was made based on a number of circumstances:

- *Accessibility*: A file that exclusively consists of a sequence of lines of the form “`parameter = value`”, possibly interspersed with comments, already is a valid Python script. Therefore, simulation specifications can be as simple or complicated as one likes. It is easily possible to let a proficient Python programmer add a very small (“level 4”) layer of Python code on top of the `Nmag` system to turn it into a very specialized tool for magnetic simulations that also is extremely simple to use by less computer literate users – e.g. for automatically producing a large number of graphs of hysteresis loops.
- *Availability*: Python is widely available, under a free license, on a large number of platforms.
- *Familiarity*: Python (unlike Lisp/Scheme) has a simple syntax that is easily picked up by anyone who has had previous exposure to virtually any other imperative programming language (such as C, Perl, Matlab, or even the shell).
- *Popularity*: Python both has a sizable user base, especially in engineering, and is rather accessible for both the inexperienced casual user and the expert.
- *Power*: Python supports enough abstract concepts (e.g. container data structures such as dictionaries) to make the implementation of more sophisticated algorithms for control and data processing a realistic option.

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<sup>13</sup>This phenomenon, which has been encountered with word processors, CAD software, ray tracers, web browsers, databases, is commonly referred to as *Greenspun's Tenth Rule of Programming*: ‘Any sufficiently complicated C or Fortran program contains an ad hoc, informally-specified, bug-ridden, slow implementation of half of Common Lisp.’

- *Engineering Relevance:* There are a number of Python libraries that make it a viable substitute for Matlab.

Python support also brings some additional secondary benefits:

- *Interactivity:* It is possible to use the Python interface in an interactive execute-commands-as-they-are-given fashion to explore and hence get a more intimate understanding of some particular system. *With Nsim, this also works for parallel computations: interactivity and parallelism do not exclude one another [32].*
- *Libraries:* There is a large number of third-party Python libraries which easily can be used to provide additional capabilities such as database support, image generation, automatic website generation, and much more.
- *Debugging:* Experienced Python programmers can utilize advanced debugging capabilities which usually are hard to find in application-specific languages. With Python, it even becomes possible to interactively inspect the situation in the context where a problem occurred by escaping to a command line from deep within the program.

However, should Python go out of fashion at some point in the future (as so many other scripting languages have done), `Nsim` is designed in such a way that it would be possible to include support for another user interface level language with reasonable implementation effort.

### 5.11.3 Python libraries

While from the perspective of a Python programmer, `Nsim` behaves like a Python library, it usually is executed as a special program that behaves like an extended Python interpreter, rather than just starting the standard Python interpreter and then importing the `nsim` module. There are a number of reasons related to the behaviour of different subsystems utilized by `Nsim` that suggest such a design. In particular, some implementations of the MPI framework use extra command line arguments to communicate parallel execution parameters which may clash with parameters used by the Python interpreter<sup>14</sup>. As this may cause some inconvenience to Python programmers, and as these issues are merely technical subtleties rather than truly fundamental limitations that would prevent `Nsim` from being turned into a proper Python extension module, this is actively being worked on at the time of this writing.

### 5.11.4 Dynamic fast code and scripting languages

One general problem inherent in a scripting language approach is that situations may arise where small pieces of user-specified code, such as e.g. a function describing a scalar potential, or a non-linear local field equation, has to be evaluated so often that only a compiled machine-code version would be sufficiently efficient not to dramatically slow down the simulation. On the other hand, it is highly desirable to retain full programming flexibility rather than artificially restricting the types of functions that can be specified.

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<sup>14</sup>This also is the reason for the existence of the `mpipython` program



There are a number of high level languages which both can be used interactively and produce fast machine code at the same time.<sup>15</sup> However, producing machine code from scripting language code is not a realistic option as scripting language popularity seems to be strongly influenced by fashion trends: one would have to tie the system so strongly to one particular user interface language that switching over to a different one becomes unrealistic. Also, in the specific case of Python, the Python compiler, Psyco [35], does not (at the time of this writing) support code generation for machine architectures other than x86-32, i.e. cannot generate fast 64-bit code.

Therefore, `Nsim` pursues a different approach: virtually all situations where user-specified pieces of code in a field theory simulation system have to be fast can be regarded as special cases of routines that implement a  $\mathbb{R}^n \rightarrow \mathbb{R}^m$  function, potentially with additional internal state, potentially utilizing an extra level of pointer indirection to get at numerical data. So, the `Nsim` simulation compiler provides capabilities to regard a user-specifiable string as a piece of C code and turn this into a callable function. Internally, this works by dynamically generating a C source file which is sent to the C compiler to produce a shared object which then is linked lazily – i.e. when such a function is used for the first time – (using the `dlopen()` and `dlsym()` functions from `libdl`) into the running simulation.

Site-wise execution of C code generated from a specification of a local polynomial in fields (such as anisotropy energy in micromagnetism) uses this mechanism in conjunction with a number of autogenerated C preprocessor macros as well as an extra array of pointers to floatingpoint data which provide access to the site-relevant field entries.

This mechanism – implemented in the `fastfields` module in the `Nsim` code – satisfies some evidently very desirable properties:

- The C compiler is not called unnecessarily: When 100 functions that have to be compiled are defined one after another before any one of them is called, only a single call to the C compiler is being made. (This is achieved by lazily deferring compilation to the latest possible point in time.)
- Whenever recompilation is initiated, functions that have become inaccessible through forgetting all references to them (i.e. they have become garbage) automatically disappear from the dynamically generated library. (So, re-defining such a function 1000 times during the course of a program will not increase memory usage.)
- At any given time, only a single dynamically compiled shared object module will be linked in. (This means that defining and calling new functions (which induces recompilation) will have to unlink and reset the symbol-to-address associations of other dynamically compiled functions (which will once again have to be looked up using `dlsym()` after relinking).)

The major drawback of the present implementation is that a single syntactic error in one user-specified C function will break all such functions (as it breaks recompilation). The most promising approach towards this problem presumably is to add an extra checking phase where the compiler is used on every single function as it is specified for the first time to find code errors and reject it (i.e. compile it to a function that raises an exception) if this situation occurs.

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<sup>15</sup>Two widely known examples would be the CMU Common Lisp compiler [33] and the SML/NJ system [34]

## 5.12 Parallelization

The capability to use parallel computation both to speed up linear algebra as well as non-linear (site-local) operations as well as to distribute the memory requirements of data structures should be considered more a necessity than merely a desirable feature. The underlying reason is that parallel computation is widely used in simulations these days, hence a nonparallel simulation framework would suffer from severely restricted applicability in view of the present range of problems studied by computer simulations. This is much more so due to the increasing availability of multicore CPUs.

### 5.12.1 The MPI execution model

Concerning parallelized number-crunching (as opposed to e.g. massive parallel lookup and search operations over clusters of potentially unreliable machines, i.e. search engine technology), the situation that emerged over the last years is strongly dominated by the availability of a flexible unified interface for efficient data exchange between processes partaking in a parallel computation, namely the MPI libraries. Very broadly speaking, MPI-based programs consist of a mixture of ‘ordinary’ commands as well as ‘collective’ commands. The role of the latter can be regarded as providing a refinement of the execution semantics of the underlying programming language (most often, C) by defining a kind of ‘must happen in unison across all processes participating in the computation’ generalized execution flow concept. Traditionally, this is usually achieved by writing MPI-based programs in such a way that all machines run the same program code which executes the same sequence of statements on all cluster nodes, very slightly seasoned only with node-number dependent range selections that ensure every process works on its share of the (often, linear algebra based) distributed workload. In particular, the entire parallel communication choreography is pre-determined right from the start of the program.

We will call this execution model the ‘choir model’: with the image in mind of songtext distributed at the beginning to all the singers which precisely defines when to sing which tune, where to loop (and how often), etc.

The obvious advantage of this model is that it is very easy to comprehend, implement, and debug. In principle, more general distributed algorithms could be (and often are!) far more complicated. For evident reasons, the choir model is the dominant model for parallelized number crunching.

Unfortunately, this kind of execution semantics is fundamentally incompatible with the idea of providing maximum user flexibility. In particular, as soon as there is any way how program flow could depend on nonpredictable external input (such as, for example, provided interactively by a human user), the choir model no longer can be applied. Instead, we must resort to a more sophisticated model where not only the data to be worked on, but also information about the nature and order of operations on that data has to be distributed at run time across all the computation nodes.

Furthermore, subtle issues arise in conjunction with dynamical distributed resource management. While memory management for conventional parallel number crunching programs usually is rather trivial, allocating all relevant data structures in the beginning, populating matrices, doing the computation, freeing all resources in the end, the situation is very different for highly dynamical applications. When does a vector which is distributed across all nodes of a cluster become inaccessible, and if this happens, how do we ensure this resource is freed in unison across all the cluster nodes?

The design decision underlying the `Nsim` compiler prototype is that the user should not at all have to worry about any issues related to parallel execution. With the present implementation, this goal has been achieved to the largest possible extent. The only parts of the system that are not fully parallelized are:

- Loading the mesh.
- Working out the partitioning of mesh vertices across cluster nodes.
- Some parts of the setup phase, most importantly working out the offset tables for local site-wise C code execution.
- Writing simulation data.
- Computations involving the compressed boundary element matrix that are based on HLib.<sup>16</sup>

All these cases raise somewhat tricky conceptual issues on the expected behaviour of a parallelized program that have to be resolved.

### 5.12.2 Mesh partitioning

The `Nsim` compiler utilizes the Metis/Parmetis [2] library to both work out node reorderings that improve the performance of sparse matrix operators as well as node partitionings across the cluster. Inter-process communication is used to distribute both complete meshes as well as associated partitioning information across all cluster nodes.

### 5.12.3 Shielding the user from MPI

The `Nsim` prototype enables the user to set up simulations that allow parallel execution without ever having to worry about any details associated with multi-machine execution flows. One particular issue is that of allowing users to debug their own code: if the complexity associated with parallel execution and collective MPI commands showed up at the user level, this would seriously interfere with the user's capability to inspect and analyze some particular situation interactively in a debugging session. Rather, the user should never have to concern himself with questions such as which statements he can execute interactively and which are forbidden as they would require coordinated execution of MPI-collective commands: things should just work as one would expect with the model of ordinary single-process execution flow in mind.

This is indeed achievable, but requires extensions to distribute not only numerical data across the cluster, but information about execution sequences as well. The basic idea is to let the master node execute the simulation script and make all the other nodes go into 'slave mode' where they receive and subsequently execute data, command sequences (akin to OpenGL display lists), and commands from the master. The commands understood by the slaves include:

- Shutdown of the system and subsequent termination of the program.

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<sup>16</sup>At the time of this writing, parallelizing HLib is actively being worked on.

- Parallel linear algebra resource allocation (for vectors, matrices, linear solvers, etc., but also for meshes, field layouts and functions that populate sparse matrices).
- Command sequence registration: a sequence of operations which manipulate distributed resources is registered under some particular name for later execution (so that later on, a command sequence can be executed across the cluster without having to employ parallel communication to send out every single command as it is executed).
- Execution of a previously registered command sequence.
- Parallel (linear algebra and command sequence) resource de-allocation.

It is important to note that, while the slave processes contain all the machine code of the core `Nsim` executable, they do not run the user's program but are driven exclusively by commands sent via MPI from the master node.

One could call this the 'organ model' (in contrast to the 'choir model') of parallel execution: the computation utilizes hardware that is spread out over a large area, and the musician has full freedom to interweave at will and from a central console both programming (using organ stops) and playing.

The implementation of the `Nsim` core internally is based on the Objective Caml system, which provides a proper substitution-aware function concept that is much more powerful than the more simplistic concept of a 'routine' (which is employed by most compiler languages, such as C, and sometimes confusingly called a 'function' there as well). In particular, OCaml supports (as an experimental but highly useful feature) the serialization of functions to strings in such a way that only the implicitly fixed contextual ('closure') parameters, but no compiled machine code, have to be sent over the network. This way, a function which was defined through parameter-fixing of a more generic function on the master node can easily be made available on the slave nodes as well. This is used e.g. to gain maximum flexibility in distributing functions over the cluster that populate sparse matrices. However, one consequence is that `Nsim` in its present form can not work on heterogeneous multi-architecture clusters, as one should not expect Objective Caml data structure serialization to be able to cross architecture boundaries.

A `Nsim` script can be either started in single-process mode

```
$ nsim simulation.py
```

or under MPI control (here, on four nodes) to execute in parallel:

```
$ mpirun -np 4 nsim simulation.py
```

Unfortunately, some MPI implementations are somewhat idiosyncratic in the way they provide parallelism to C programs: what effectively happens is that another pre-startup layer gets wrapped around the program's `main()` function that parses and interprets MPI-related command arguments. This is then used in conjunction with a utility for remote login (such as `ssh`) for automated coordinated startup of individual processes. This has the unfortunate effect that it can interfere with argument parsing of scripting language interpreters, such as Python.

It is important to note that the startup code of the standalone `Nsim` executable has to discern between a number of different situations: using `Nsim` to run a user simulation

program whose filename is given as a command argument induces a different startup mode than starting `Nsim` interactively. Furthermore, both interactive and script mode may be used when running `Nsim` in a distributed fashion under MPI control. (Interactive MPI-based parallel execution is a highly uncommon feature, but possible with `Nsim`.) Note that in parallel computations, regardless of whether script or interactive mode is invoked, slave processes will always go through special startup code to enter slave mode.

#### 5.12.4 Centrally coordinated parallel linear algebra

The ‘organ’ execution model described in the previous section requires the distribution and management of both linear algebra resources (vectors, matrices, linear solvers) and control resources (execution sequences of linear algebra operations). For the `Nsim` prototype, the MPI-based PETSc library was chosen to provide parallel linear algebra capabilities. In MPI parlance, PETSc creates an own communicator data structure to separate its own parallel communication from other MPI-based communication the program may also have to perform. The `Nsim` core uses an additional communicator for its own coordination and management-related messages.

The most important issue with dynamic parallel execution is dynamic resource management: both Python and the Objective Caml system provide automatic resource de-allocation capabilities (of different sophistication) that have to be extended to parallel resources. Fortunately, it is not necessary to address the interplay of Python’s dynamical memory management with parallel resources, as all parallel resources can be managed internally by the OCaml system and proper behaviour with respect to Python code is then induced automatically through the Python-OCaml interface.

The basic idea underlying dynamical resource management is that, as the master node has the sole responsibility for execution flow, garbage collection on the master node will be the sole authority on dynamic de-allocation of distributed resources. This is effected through addressing all distributed resources in an uniform way through *dynamic resource handles* which basically represent names of dynamical resources to which a finalizing function is associated – on the master machine only – that will be executed upon garbage collection. Every process participating in a parallel computation (including the master) maintains a dictionary that maps dynamic resource handles to the actual resources (i.e. this machine’s share of a distributed vector, matrix, or a distributed script, etc.) When one dynamical resource (i.e. a command sequence) refers to another one (i.e. a vector), it does so by using this dynamical resource handle, so garbage collection of the command sequence resource can induce the de-allocation of other resources referred through it.

On the slave nodes, dynamic resource handles are nothing but just keys into a dictionary containing the corresponding resources, without finalizers attached. They are being managed (i.e. allocated and de-allocated) exclusively according to resource management commands received from the master. Here it is important to know that the OCaml data serializer works in such a way that turning an entity such as a distributed resource handle into a string and sending it over the network will strip it from its finalizers. Hence, parallel command sequences can be serialized and distributed from the master to the slave processes conveniently without having to worry about spurious finalizers being introduced on the slaves.

On the master, de-allocation of a distributed resource has to induce sending out the corresponding de-allocation commands to the slave nodes, as this may involve the execu-

tion of collective MPI commands. As garbage collection can and will happen at arbitrary points throughout the execution of a program, for example in the middle of a registered sequence of linear algebra commands which involves MPI-collective operations before and after the garbage collection, the master *must not* induce distributed de-allocation from within a distributed resource handle finalizer (as this may upset the synchronicity of the sequence of MPI-collective commands across machines), but instead defer the actual sending of de-allocation requests to the next point in time when slaves are again ready to receive commands from the master. The obvious drawback of this approach is that there are situations where distributed resources refer to other distributed resources in such a way that de-allocation cannot happen simultaneously but will artificially be spread out over multiple cycles of garbage collections and entries to the parallel command distribution code. For real world applications, however, this does not pose a problem.

Evidently, the resource tables that map distributed resource handles to the actual resources must not use those actual distributed resource handles as keys for which finalizers were registered (otherwise their presence in these tables would prevent them from ever being collected!) While one may employ weak reference tables to circumvent this problem, a simpler approach is to use copies of the distributed resource handles as table keys which do not have finalizers registered.

### 5.13 On the implementation of Nsim’s core capabilities

Underneath the user interface, Nsim has to provide not only numerical capabilities, but also some rather sophisticated bookkeeping as well as symbolic transformations (e.g. analytically working out integrals over simplices). Evidently, it is highly desirable to have these computationally demanding parts implemented in a fast compiler language. The major criteria that influence the choice of a viable compiler to base such a system (developed in an academic environment) on are:

- The compiler should be sufficiently well supported to get feedback from the developer team when low level technical issues (such as interaction with MPI) arise.
- The compiler should be able to produce efficient code for the most widespread platforms.
- The language should provide basic capabilities that are highly useful when implementing symbolic algorithms, including lambda abstraction, closures, tail recursion, and a proper garbage collector.
- The language should be sufficiently easy to pick up for new PhD students on the project (which may be physicists or engineers rather than computer scientists), so that they can start to be productive very early on.
- The language should allow interfacing specialized C libraries (e.g. for parallel sparse matrix linear algebra) without too much effort.

The Nsim authors found that the Objective Caml system satisfies these criteria very well. In addition, when the implementation of the Nsim compiler started, there already was an OCaml-Python interface available [36] that provided a very tight coupling between the chosen user interface and the core implementation language, even to the extent of



making it possible to wrap up OCaml functions to make them callable from Python and vice versa. The implementation of `Nsim` only uses a subset of OCaml language features which is what is known as ‘Core ML’ plus a few extensions. The underlying reason is that this subset of the full language on the one hand already is sufficiently powerful to tackle practically all problems that arouse in the implementation of `Nsim`, and on the other hand is sufficiently simple to be mastered by students within about three months. As an additional benefit, this voluntary restriction greatly simplifies porting `Nsim` to Microsoft’s F# [37].<sup>17</sup>

During the implementation of the `Nsim` prototype, the original ‘Pycaml’ module (which also is readily available as ‘pycaml’ package in the popular Debian GNU/Linux distribution) was extended considerably by introducing new functions to simplify writing Python extensions in OCaml. Also, a number of memory management related problems had to be fixed (both on the Python and OCaml side). One of the strongest benefits of this module is that it ‘magically’ handles all memory management related issues that have to be addressed in order to make the OCaml garbage collector and Python reference counting mechanism collaborate. This is a short example that demonstrates how to extend Python with a fast (i.e. compiled to machine code) implementation of Euler’s Gamma function  $\Gamma(x)$  based on extended Pycaml:

```

=== OCaml ===

let rec euler_gamma =
  (* Accurate to eps_rel = 2e-10; See http://www.rskey.org/gamma.htm *)
  let pi = 4.0*(atan 1.0) in
  let constants =
    [|75122.6331530; 80916.6278952; 36308.2951477;
      8687.24529705; 1168.92649479; 83.8676043424;
      2.50662827511|]
  in
  let nr_constants = Array.length constants in
  fun x ->
    if x<0.0
    then -.pi/(x*(euler_gamma (-.x))*(sin (pi*.x)))
    else
      let rec compute_sum_prod sum prod pow_x n =
        if n=nr_constants then sum/.prod
        else
          compute_sum_prod
            (sum+.constants.(n)*.pow_x)
            (prod*(x+(float_of_int n)))
            (pow_x*.x) (n+1)
      in
      let x5 = x+.5.5 in
      exp(-.x5)*(x5**(x+.0.5))
      *(compute_sum_prod 0.0 1.0 1.0 0)
  in
let _py_gamma =
  python_interfaced_function [|FloatType|]
  (fun py_args ->
    pyfloat_fromdouble (euler_gamma (pyfloat_asdouble py_args.(0))))

```

<sup>17</sup>At the time of this writing, this is actively being worked on, with rather encouraging intermediate results: a non-parallel F#-based port of the `Nsim` framework has been demonstrated in summer 2009 by M. Franchin [38].

```

in
  register_for_python [|("gamma",_py_gamma)|]
;;

=== Python ===

>>> ocaml.gamma(0.5)
1.7724538509046035
>>> math.sqrt(math.pi)
1.7724538509055159

```

## 5.14 Performance

Comparison of the `Nsim`-based micromagnetic application `Nmag` with another finite-element based micromagnetic package that uses very similar technology (i.e. the same time integrator and linear algebra libraries) allows us to get an idea of the performance of the generic approach towards simulations relative to tailored C code. Internally, the structure of the computations done in the main simulation loops of `Nmag` and the finite element based micromagnetic simulator `Magpar` [39] are very similar, up to minor technical details such as the question how to enforce the length constraint on magnetization vectors and how to do residual gauge fixing. One finds that for a given system, the time spent in the main simulation loop for `Nmag` and `Magpar` usually differs by less than 20% in either direction. However, both setup time and memory requirements are presently noticeably larger for `Nmag` than for `Magpar`. Concerning the setup phase, this is strongly expected, as the technology presently underlying `Nsim` resembles that of a ‘bytecode interpreter’ for linear operator descriptions, while `Magpar` uses hand-written compiled C code to initialize its operator matrices. Presently, the `Nsim` prototype needs about 60% more memory for internal bookkeeping than `Magpar` on simulations that are reasonably large to be of practical relevance. There is strong evidence that this overhead is caused by technicalities in the setup phase and can be brought down quite considerably.

## 6 Limitations

The approach towards simulation physics underlying the `Nsim` framework has limitations of different nature: fundamental limitations that cannot be overcome, conceptual limitations where it is as yet unclear which approach is the most promising one, as well as technological restrictions that can (and most likely eventually will) be overcome. As misconceptions about which problem belongs to which category occasionally arise, it makes sense to give a short list of the most relevant issues.

### 6.1 Fundamental limitations

Numerical simulations based on unstructured (simplicial) finite element meshes naturally involve a considerable bookkeeping overhead to keep track of the structure and topology of both the mesh as well as linear operators. Hence, memory requirements are a more constraining factor here than with finite difference based simulations and put a stronger limit on the maximal number of degrees of freedom that can be included in a simulation. While much of the underlying structure of `Nsim` could be extended rather easily to

support finite differences and structured meshes in addition to finite elements, the fundamental limitation of increased memory requirements for unstructured finite element based approaches cannot be overcome.

## 6.2 Conceptual limitations

While most of the pieces for a simple unified description language for physical systems have been implemented, this has not yet been integrated in such a way that a parallel simulation can be produced from a single textual description file. Rather, the specification has to be done piece-wise for individual parts such as differential operators, local field operations, etc. Technically speaking, this can be easily overcome by combining these pieces into a unified LALR(1) grammar. However, some unresolved conceptual issues include finding a suitable (i.e. convenient) notation for computations which presently have to be specified as sequences of linear algebra operations (such as for the computation of the demagnetizing field in micromagnetism).

By implementing both support for key techniques in conjunction with convenient notational conventions, a simulation framework can gain considerable expressive power and broad applicability. From the perspective of renormalization theory, we would expect situations to be rare where a field theoretic model has to employ concepts beyond these:

- Differential operators of order 1 and 2.
- Local (i.e. nondifferential) non-linear operators.
- Fields mediated by very light or massless particles which give rise to ‘Coulomb’s Law’ type interactions.

However, this perspective leaves open many important questions on what approach to discretisation will behave how well or how badly.

## 6.3 Technical restrictions of the `Nsim` prototype

For the purpose of providing an overview, we summarize the most relevant open issues that at the time of this writing have not been implemented in the public release of the `Nsim` prototype. Most of these have been described in more detail in the preceding text.

- The `fastfields` dynamic linking mechanism at present easily gets confused if it is ever fed broken C code. Ideally, calling a dynamically compiled function for which a broken definition was given should throw an exception which contains both the compiler error message and some context from the code provided by the user. This is achievable, but has not been implemented yet.
- Error reporting can (and eventually must) be improved considerably. At present, there are still a few situations where a minor mistake in a simulation specification can produce a highly cryptic error message (such as “index out of bounds”) that is hard to track down.
- Support for dynamic rebuilding of sparse and nonsparse operator matrices as well as the inclusion of ‘middle fields’ still is fragmentary in the public release.

- At present, field dependencies must be specified by the user. While it would be rather straightforward to auto-derive the field dependencies from the specifications of the linear algebra execution sequences as well as the user-specified local equations, this has not been implemented yet.
- Startup argument handling of `Nsim` still is rather ad-hoc. Basically, there are six different kinds of program arguments that have to be dealt with:
  - MPI startup arguments
  - PETSc related arguments
  - Arguments controlling the Python interpreter
  - `Nsim` arguments (controlling e.g. the `nsim` loglevel)
  - `Nsim` library arguments (e.g. when using the `Nmag` library)
  - Arguments to the user’s application/script.

The `Nsim` team has a strategy for eventually handling this complexity in a convenient way, but this has not been implemented yet.

- An important limitation of the extended Pycaml Python-OCaml interface module (to be released separately as a spin-off of the `Nsim` project) is that it is not thread-safe with respect to Python threads. While this has no relevance to the `Nsim` project at present, the wider community may nevertheless benefit from making this module thread-safe.
- A major re-structuring of the code that auto-generates the Jacobian from the equations of motion has not been fully completed yet.
- `Nsim` does not support complex-valued fields (and operators), as the PETSc library cannot handle both complex and real vectors at the same time. In order to resolve this, one would most likely have to wait for a major change to the PETSc library or find a way to compile it in such a way that two variants (which use different symbol prefixes) can be linked at the same time, one for real valued computations, the other one for complex computations (which then would most likely use different MPI communicators).
- `Nsim` presently neither supports dynamic mesh refinement nor non-simplicial mesh geometries. (Considering refinement, this is considered to be difficult to get right in micromagnetism, avoiding numerical artefacts.)

## 7 Conclusion and outlook

The viability of automated compilation of symbolically specified physical simulations to fast parallel code in a way that preserves user-level sequential computing semantics has been demonstrated through `Nsim`. Furthermore, the practicability of such an approach as a basis for simulations of scientific relevance also has been demonstrated through the micromagnetism library `Nmag` implemented on top of `Nsim`. As practicality and usability are the main driving forces underlying the design of the `Nsim` framework, many strategic

decisions were relentlessly revamped (sometimes multiple times) whenever the authors discovered that an early design decision had led to more inconvenience in usage than was originally expected. As such, much of the design of `Nsim` must still be considered a ‘moving target’ that has not stabilized in its final form yet. But for precisely this reason, malleability of the higher levels close to the end user, it is considered important to inform the wider academic community of the status of this project at the present state and utilize the academic process to guide further design decisions – now that the structure of the system’s simulation core has stabilized – in those directions most useful for applications.

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## A A complete `Nsim` example

An example for level 3 Python user code on top of the `Nmag` micromagnetic library has been given in figure 2. This appendix provides a complementary level 2 Python example that shows how to employ the concepts described in the main body of this work to set up and simulate a complete physical model that involves PDEs. Also, it shows how to combine a `Nsim` simulation with other software libraries for setup, data analysis, and plotting. While the simulation script is essentially a sequential program, it can be started in parallel on a cluster and will then utilize MPI-based linear algebra to distribute the simulation-related computational effort across nodes. The data analysis part always gets executed as sequential code on the master node.

### A.1 The physical system

The system to be studied is a reaction-diffusion system that was originally proposed by Alan Turing as a model for morphogenesis in biological systems [40]. While the framework provides all the bookkeeping infrastructure (as explained in the main part of this work), the level 2 interface of `Nsim` is still somewhat rudimentary at the time of this writing, and could be simplified considerably by adding more inference logic and introducing a dedicated grammar that can be used to express a complete task specification: with this, it should be possible to bring down the programming effort required to specify the physics

of a field theoretic system like the one presented here from presently about 75 lines to less than 20. One reason for the present redundancy is that, during `Nsim`'s evolution, major design changes have occurred, such as the replacement of the original parallel timestepper functionality with new code that is more tightly integrated with the main part of the simulation. Such low-level structural changes favor some independence in higher-level specifications, which here shows up as redundancy.

The system under study can arise as a linearization around a stationary point of a binary chemical system whose position-dependent concentrations  $u(x, y)$ ,  $v(x, y)$  change according to:

$$\begin{aligned}\frac{d}{dt}u &= f_u(u, v) + D_u\Delta u \\ \frac{d}{dt}v &= f_v(u, v) + D_v\Delta v.\end{aligned}\tag{15}$$

Let us assume that the truncated system that is obtained by setting the diffusion constants  $D_u = D_v = 0$  has a stationary point at  $(u_0, v_0)$ . Then, the linearized system that is obtained by taking the  $\epsilon \rightarrow 0$  limit of  $u = u_0 + \epsilon\tilde{u}$ ,  $v = v_0 + \epsilon\tilde{v}$  is governed by the equation

$$\frac{d}{dt}\begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = \left( \begin{array}{cc} \frac{\partial f_u}{\partial u} & \frac{\partial f_u}{\partial v} \\ \frac{\partial f_v}{\partial u} & \frac{\partial f_v}{\partial v} \end{array} \right)_{|(u_0, v_0)} \cdot \begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} + \begin{pmatrix} D_u\Delta\tilde{u} \\ D_v\Delta\tilde{v} \end{pmatrix}.\tag{16}$$

If a number of conditions on the diffusion constants and the matrix of partial derivatives are satisfied, then the situation can arise that the system's stability with respect to spatially oscillating fluctuations of the form

$$(\tilde{u}(\vec{x}), \tilde{v}(\vec{x})) = (\tilde{u}_*, \tilde{v}_*) \cdot \cos(\vec{k} \cdot \vec{x})\tag{17}$$

is violated for some range of wave-vectors  $\vec{k}$  with  $k_{\min} < |\vec{k}| < k_{\max}$ . Over this range of wave-vectors, initial random fluctuations get amplified, which leads to the formation of patterns, as shown in figure 5.

The parameters chosen for this example are:

$$\left( \begin{array}{cc} \frac{\partial f_u}{\partial u} & \frac{\partial f_u}{\partial v} \\ \frac{\partial f_v}{\partial u} & \frac{\partial f_v}{\partial v} \end{array} \right) = \begin{pmatrix} +1 & +2 \\ -2 & -3 \end{pmatrix}, \quad D_u = -0.025, \quad D_v = -0.25\tag{18}$$

on a disk with radius  $R = 10$ . Note that the trace of the linearization matrix is negative, while the determinant is positive, so the realparts of the eigenvalues are negative, and the system is stable in the long wavelength ( $k \rightarrow 0$ ) limit. For intermediate values of  $|\vec{k}|$ , the negative contribution to the determinant from the diagonal entries over-compensates the positive off-diagonal contribution to the determinant, so the determinant becomes positive while the trace remains negative, i.e. one of the two eigenvalues will obtain a positive real part, which causes the instability. For large  $|k|$ , the diagonal again gives a large positive contribution, and the realparts of the eigenvalues are negative again.

## A.2 The Python code

The complete Python program that produced this output is given in the following. The central part that sets up the physics simulation engine is the call to `make_linalg_machine()`. This translates a full specification of field layouts, linear operators, local reaction equations, short sequences of elementary parallelizable operations, and numerical tweaking parameters to an opaque object that can be used to perform time integration in such a



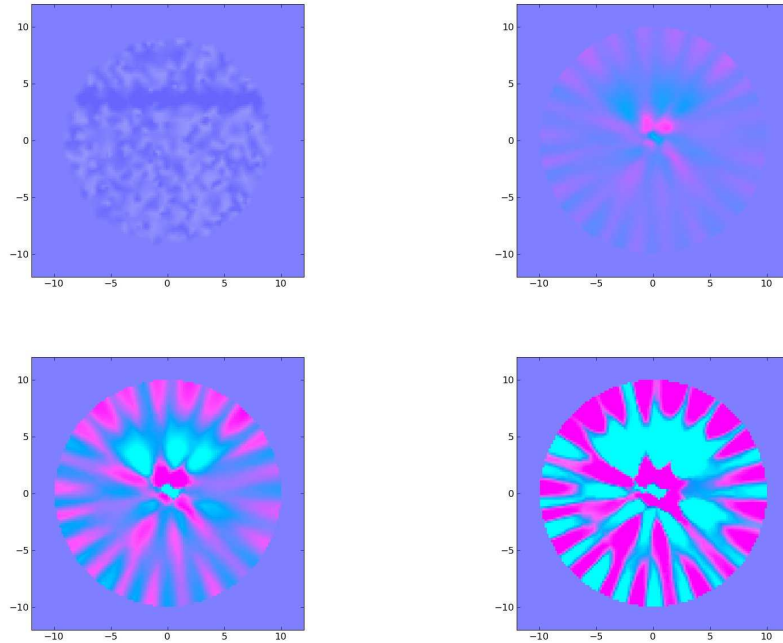


Figure 5: Pattern formation from random initial noise by the Turing instability in a reaction-diffusion system.

system. The part of the code starting with the `sample_field()` function deals with data extraction and visualization only.

```
import math, numpy
from nsim.linalg_machine import *

# Work around a memory management problem of pylab:
import matplotlib
matplotlib.use('Agg')
import pylab

(R_disk,s_disk) = (10.0, 0.5)
n_boundary=int(1+2*math.pi*R_disk/s_disk)
n_interior=int(1+math.pi*R_disk**2/(s_disk**2))

disk_boundary=[[R_disk*math.cos(2*math.pi*n/n_boundary),
                R_disk*math.sin(2*math.pi*n/n_boundary)]
               for n in range(n_boundary)]

# Generate a mesh - this will just have one material region,
# whose number is 1. (This mesh-generating function gives fairly
# poor results and is supposed to be used for testing purposes only!)
mesh_disk=ocaml.simple_convex_mesh(disk_boundary,0,n_interior,10)

# Generate a postscript file that shows the 2d mesh:
ocaml.mesh2d_ps(mesh_disk, "/tmp/disk%d.ps"%n, [10.0,10.0,200.0,200.0])

(elem_dim,elem_order)=(2,1)
elem_uv = ocaml.fuse_elements(\
    ocaml.make_element("u", [], elem_dim, elem_order),
```

```

ocaml.make_element("v", [], elem_dim, elem_order))

mwe_uv = ocaml.make_mwe("uv", mesh_disk,
                        [(0, ocaml.empty_element), # "vacuum"
                         (1, elem_uv)], [], [])

mwe_uv_dot = ocaml.mwe_sibling(mwe_uv, "uv_dot",
                               "d_dt_", # element renaming prefix
                               [("u", "u_dot"), ("v", "v_dot")])

mwe_uv_diff = ocaml.mwe_sibling(mwe_uv, "uv_diff",
                                "Diffusion_",
                                [("u", "u_diff"), ("v", "v_diff")])

# Equations of motion:
eq_ydot = ""
u_dot <- u_diff + (+1.0)*u + (+2.0)*v;
v_dot <- v_diff + (-2.0)*u + (-3.0)*v; ""

the_lam=make_linalg_machine("Turing",
                             mwe=[mwe_uv, mwe_uv_dot, mwe_uv_diff],
                             vectors=[lam_vector(name="v_uv", mwe_name="uv"),
                                       lam_vector(name="v_uv_dot", mwe_name="uv_dot"),
                                       lam_vector(name="v_uv_diff", mwe_name="uv_diff")],
                             operators=[\
    lam_operator("op_diff", "uv_diff", "uv", \
    "-0.025*<d/dxj u_diff||d/dxj u>\
    +(-0.25)*<d/dxj v_diff||d/dxj v>, j:3)],
                             local_operations=[\
    lam_local("local_uv_dot",
              field_mwe=["uv_dot", "uv_diff", "uv"],
              equation=eq_ydot)],
                             programs=[\
    lam_program("set_uv_diff",
                commands=[["SM*V", "op_diff", "v_uv", "v_uv_diff"],
                           ["CFBOX", "uv_diff", "v_uv_diff"]]),
    lam_program("update_uv_dot",
                commands=[["GOSUB", "set_uv_diff"],
                           ["SITE-WISE-IPARAMS", "local_uv_dot",
                            "v_uv_dot", "v_uv_diff", "v_uv"], []]),
    ],
                             timesteppers=[
    lam_timestepper("TS", \
    ["uv", "uv_dot", "uv_diff"],
    ["v_uv", "v_uv_dot", "v_uv_diff"],
    "update_uv_dot",
    nr_primary_fields=1,
    pc_rtol=1e-8, pc_atol=1e-8,
    max_order=2, krylov_max=5,
    jacobi_eom=eq_ydot,
    phys_field_derivs=[("PRIMARY", ""),
                       ("PRIMARY", ""),
                       ("OPERATOR", "op_diff")],
    jacobi_prealloc_diagonal=50,
    jacobi_prealloc_off_diagonal=50)])

```

```

def advance_time(field,times,do=None):
    t_initial=times[0]

    ocaml.linalg_machine_set_field(the_lam,field, "v_uv")
    ocaml.linalg_machine_initialize_timestepper(\
        the_lam,"TS", t_initial,
        1e-7,1e-7) # rel and abs tolerances
    n=0
    if do: do(field_uv,t_initial,n)
    for time in times[1:]:
        ocaml.linalg_machine_advance_timestepper(\
            the_lam, "TS", time,
            1000000) # max iterations
        n=n+1
        ocaml.linalg_machine_get_field(the_lam,field,"v_uv")
        if do: do(field_uv,time,n)
    return field

def sample_field(field,radius,npoints=128):
    v=numpy.zeros([npoints,npoints,2])
    step=2*radius/(npoints-1.0)
    min_coord=-step*(npoints-1.0)/2.0
    coord_range=[min_coord+n*step for n in range(npoints)]
    for yc in range(npoints):
        for xc in range(npoints):
            pos=[coord_range[xc],coord_range[yc]]
            z=ocaml.probe_field(field,"u",pos)
            # z is e.g. [('u', 37.511166751728595)], or []
            if len(z)>0:
                v[yc,xc,0]=z[0][1]
                z=ocaml.probe_field(field,"v",pos)
                v[yc,xc,1]=z[0][1]
    return (v,-min_coord)

def plot_sampled(sampled,color_range=1.0):
    pylab.hold(False)
    for nr_plot in range(len(sampled)):
        print "Doing plot:",nr_plot
        (data,xmax)=sampled[nr_plot]
        npoints=data.shape[0]
        cdata=numpy.zeros([npoints,npoints,4],dtype=numpy.uint8)
        for yc in range(npoints):
            for xc in range(npoints):
                u=data[yc,xc,0]
                v=data[yc,xc,1]
                red=int(255*(0.5+u/color_range))
                green=int(255*(0.5+v/color_range))
                red=max(0,min(red,255))
                green=max(0,min(green,255))
                cdata[yc,xc]=(red,green,255,255)
            pylab.imshow(cdata,
                interpolation="nearest",
                extent=(-xmax,xmax,-xmax,xmax))
        pylab.savefig("/tmp/turing%02d.png"%nr_plot)

def fun_uv(dof,pos):

```

```

"""This function produces some initial all-wavelength 'noise'"""
(dof_stem,dof_indices)=dof
if pos[0]*pos[0]+pos[1]*pos[1]>80.0:
    return 0.0 # No fluctuations close to the boundary
# Pseudo-Random fluctuations otherwise:
return (((((4*math.pi+pos[0])**8)%1.0+\
          math.pi+pos[1])**8)%1.0-0.5)*1e-3

field_uv=ocaml.raw_make_field(\
    mwe_uv, [fun_uv], # opt. sampling fun
    "", "")

plots=[]

def do_add_plot(field,time,n):
    print "\n*** DOING T=%.3f ***\n"%time
    plots.append(sample_field(field,1.2*R_disk))

advance_time(field_uv,[x*50.0 for x in range(4)],
             do=do_add_plot)

plot_sampled(plots,color_range=5e-3)

```

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