tetmag – An open-source finite-element software for micromagnetic problems

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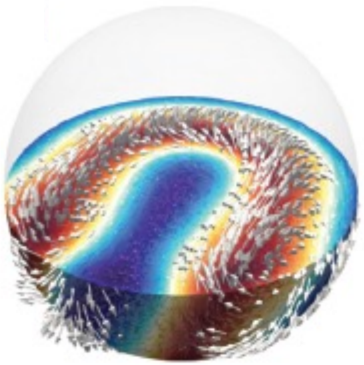

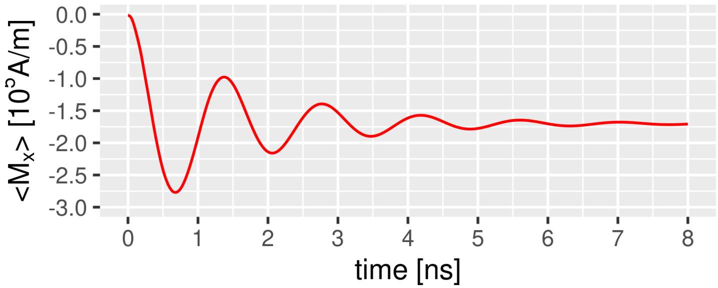

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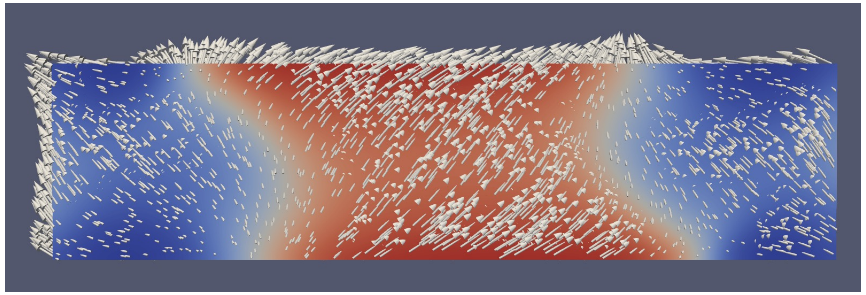
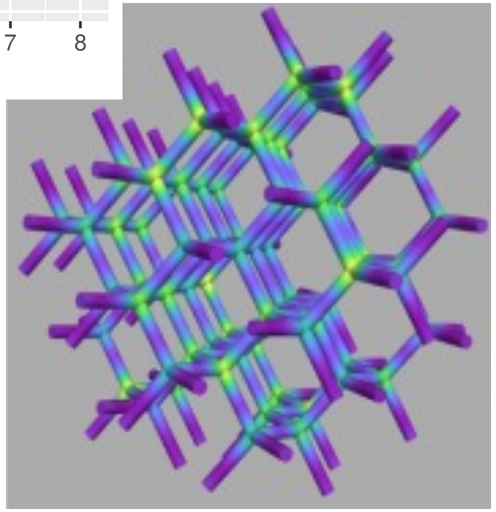




Rencontre sur les
logiciels libre de recherche
5 octobre 2023
IPCMS Strasbourg

Purpose, applications, and background of tetmag

General scientific context

- Micromagnetic theory
- Ferromagnetism on the nanoscale
- Picosecond magnetization dynamics
- Magnetization structures in nano-elements
- Spintronics
- Magnonics

https://github.com/R-Hertel/tetmag

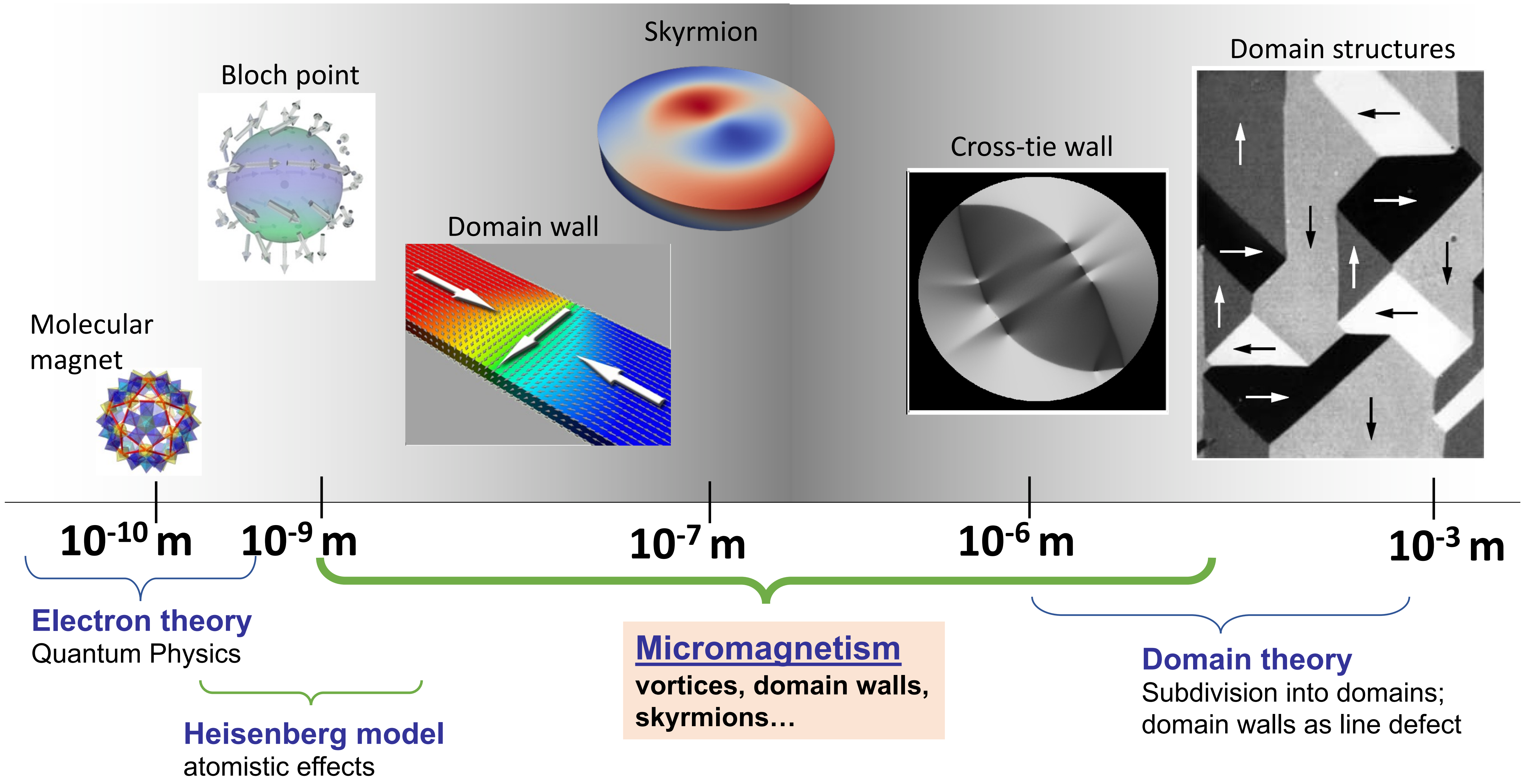
Scientific background

- Internationally renowned team with more than 25 years experience in micromagnetic theory & simulation
- Predecessors of this code were developed at Max-Planck-Institute Halle and Forschungszentrum Jülich
- Software has been used in > 100 high-impact publications
- Numerous predictions of fundamental phenomena with our simulations:
  spin wave logics (2004), magnetic vortex-core switching (2007), curvature-induced magnetochirality (2010)
- First GPU-accelerated finite-element micromagnetic software
- Finite element method for general geometries (curved or inclined surfaces, complex 3D geometries…)

Publication

First release of tetmag as open-source software in May 2023.

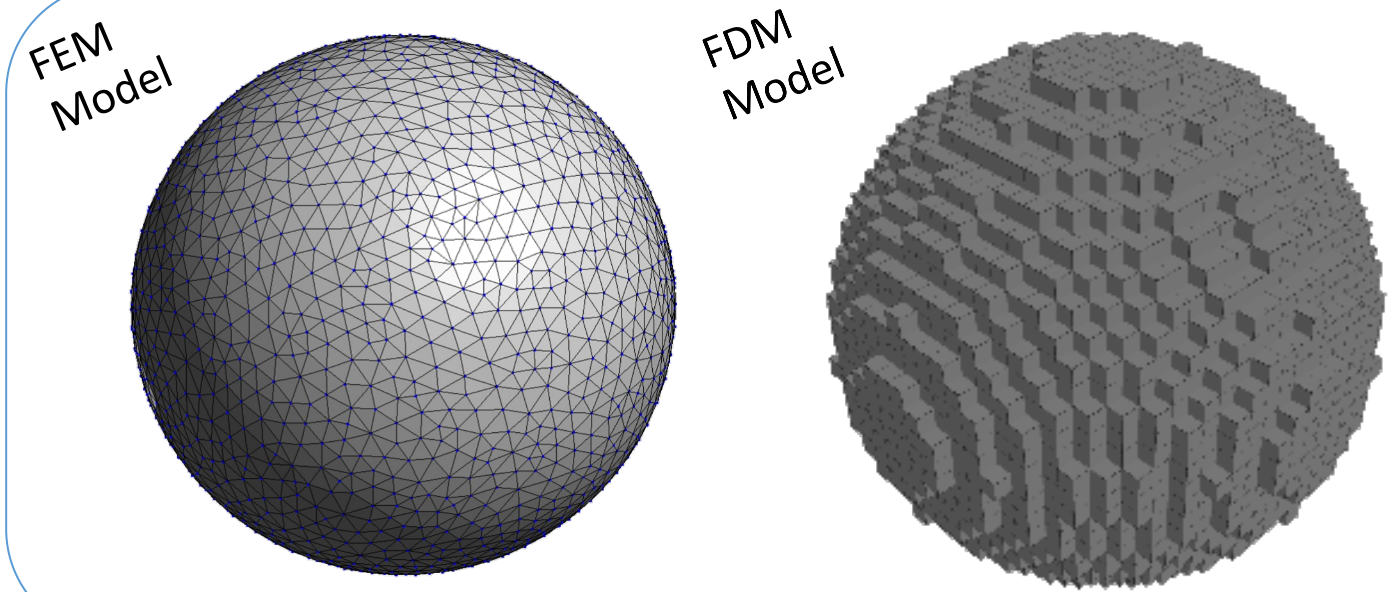
Micromagnetism: Length Scales



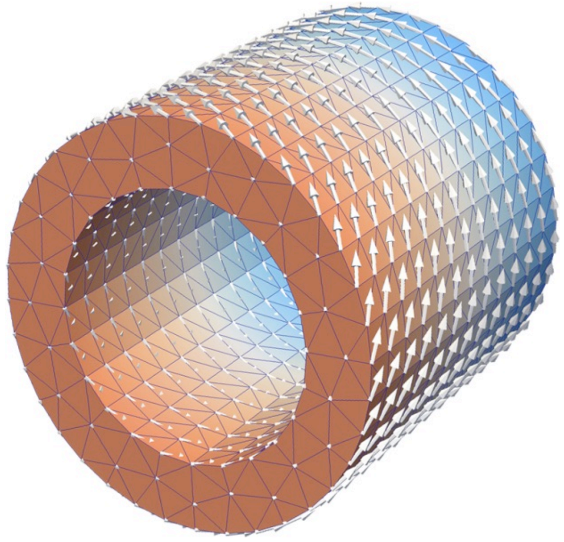
Finite Elements for Geometric Flexibility

Advantages of Finite Difference Method	Advantages of Finite Element Method
Relatively easy to implement	Accurate approximation of non-trivial geometries
Low memory requirements per DOF	Adaptive mesh refinement
fast and easy to parallelize	Well suited for three-dimensional nanostructures

Details of the sample shape can have an impact on the magnetic properties.
Geometric effects, like curvature-induced asymmetries, require precise geometric models.



C. Abert, Eur. Phys. J. B 92, 120 (2019)



Challenges in Modeling: Three-dimensional magnetic nanostructures

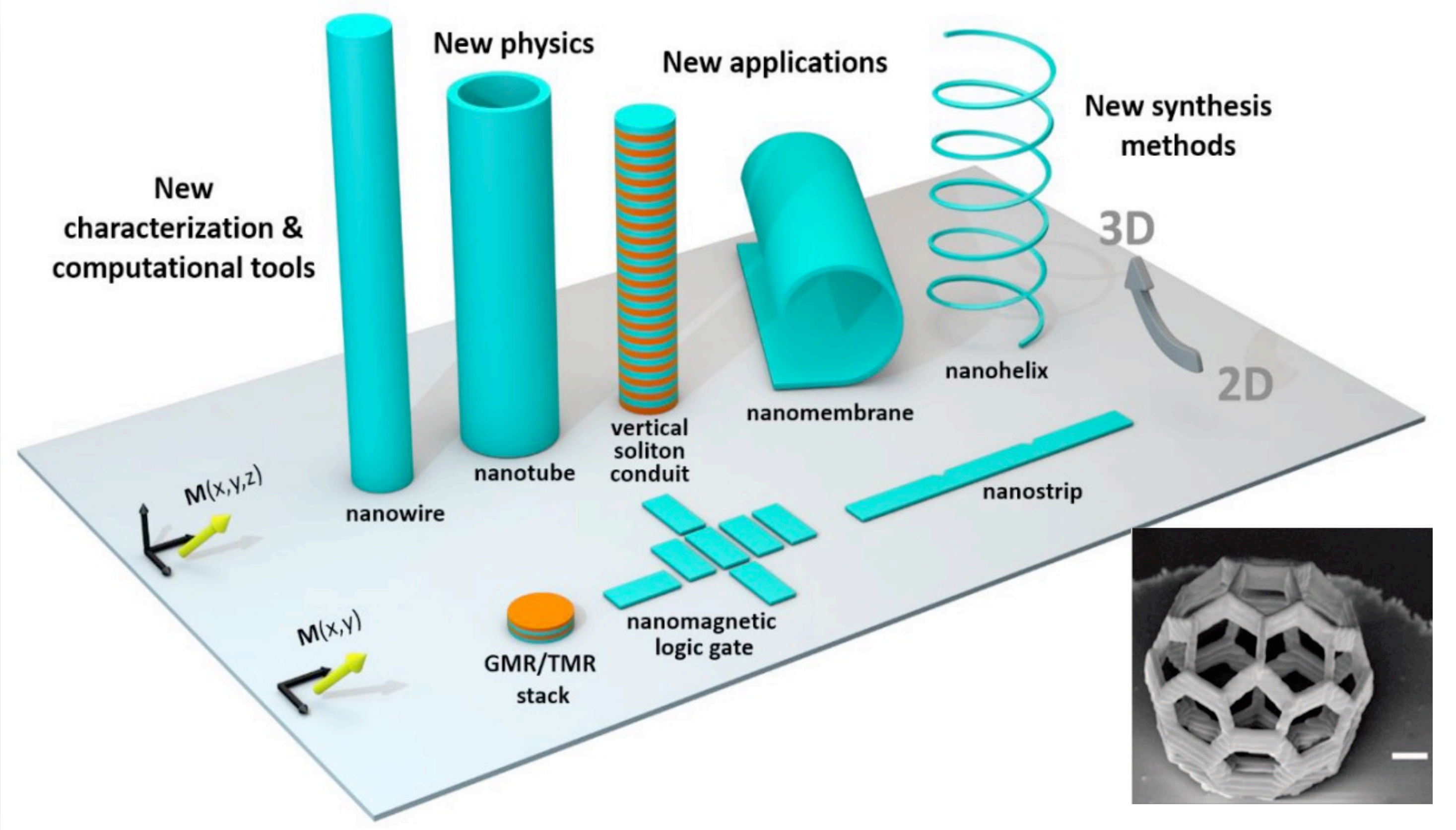
Recent development in nanomagnetism :

Three-dimensional nanostructures with complex shapes

Functionality, physical properties may depend sensitively on the shape of the nanostructure

Fernandez-Pacheco et al.
Nature Comm. 8, 15756 (2017)

Large scale problems with nontrivial geometries
Finite-element simulation with millions of elements
Typical situations in **3D nanomagnetism** • Large samples of complex shape • Arrays of interacting particles



Features of tetmag

https://github.com/R-Hertel/tetmag

Features

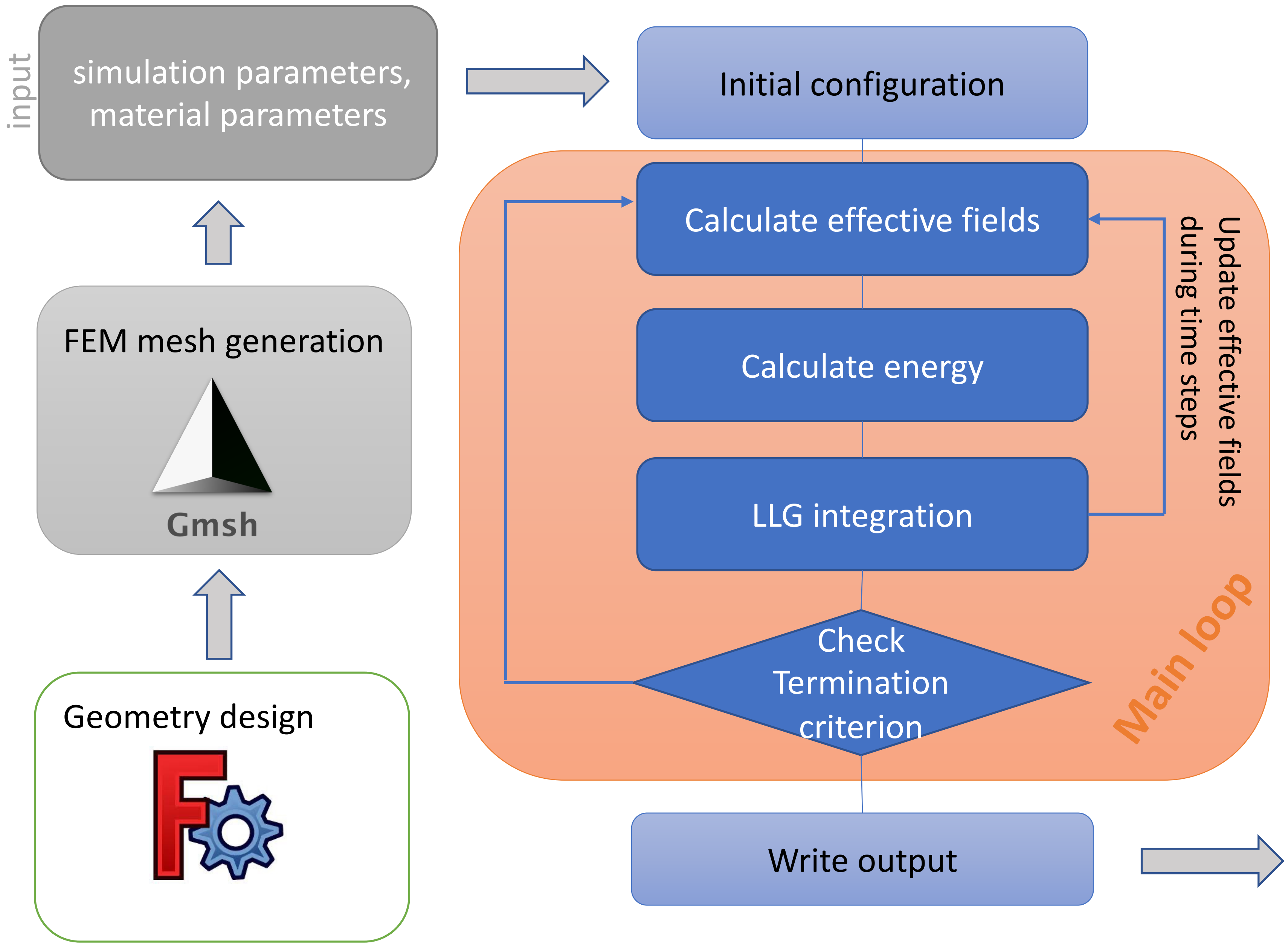
- General-purpose micromagnetic simulations with LLG + STT
- FEM for geometric flexibility
- Object-oriented C++
- Hybrid FEM-BEM calculation of magnetostatic field calculation
- H2-type matrix compression for efficient BEM integration
- GPU acceleration with CUDA / THRUST
- Platform-independent - tested on Linux and MacOS

Can treat any common micromagnetic simulation task:

- Static magnetization structures
- Magnetic switching processes
- Field-driven dynamics
- Current-driven dynamics
- Hysteresis loops

Uses several efficient libraries and tools

tetmag workflow



Repeated evaluation of effective fields in the main loop

Typical parameters:

- LLG integration time step < 1ps,
- Simulation time ~ 10 ns
- Approx. 10^5 of DOF

Millions of effective-field evaluations

Efficient algorithms required, especially for large-scale problems

https://github.com/R-Hertel/tetmag

tetmag documentation

https://tetmag.readthedocs.io

- Installation guide
- General introduction
- Examples

  Step-by-step description of simulation studies

tetmag.readthedocs.io

Ex. 3: Current-induced dynamics

When an electric current flows through a ferromagnetic material, it aquires a spin polarization through which the conduction electrons interact with the magnetization. This effect is described by the so-called spin-transfer torque (STT). In this example, we simulate the STT-induced magnetization dynamics in a square Permalloy platelet. The micromagnetic problem simulated here is based on a proposal by Najafi et al., published in Ref. 1 .

The sample is a Permalloy platelet of 100 nm $\times$ 100 nm $\times$ 10 nm size. We use FreeCAD to define the geometry and to generate an irregular FEM mesh with the netgen plugin. In our example, the mesh size is set to 2 nm, resulting in 39 246 irregularly shaped terahedral finite elements.

Calculating the initial configuration

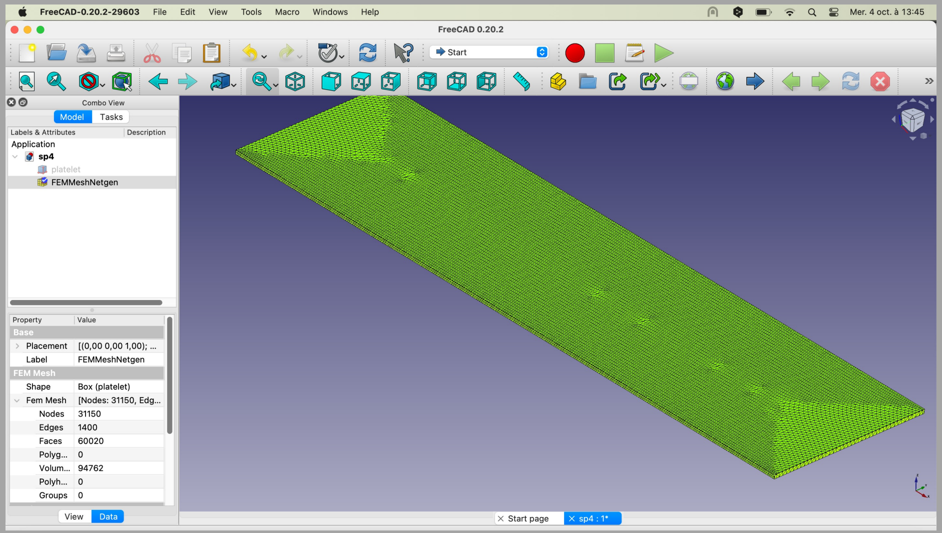
First we simulate the initial configuration – a vortex structure at zero external field and without spin-polarized current. The keyword `intial state = vortex_xy` can be used to generate a vortex-type initial structure, circulating in the xy plane, from which the magnetization can be relaxed. The `simulation.cfg` for this static part of the simulation is

```
name = sp_stt
scale = 1.e-9
mesh type = vtk
alpha = 1
initial state = vortex_xy
time step = 2 # demag refresh interval in ps
duration = 5000  # simulation time in ps
solver type = gpu
torque limit = 1.e-4
remove precession = yes
```

By performing the static simulation, we quickly obtain the converged state, stored in the file `sp_stt.vtu`, which we rename to `sp_stt_vortex.vtu`. This will be the initial state of the

tetmag in action

1. Define geometry and FEM mesh (FreeCAD)



2. Supply input data (ASCII file)

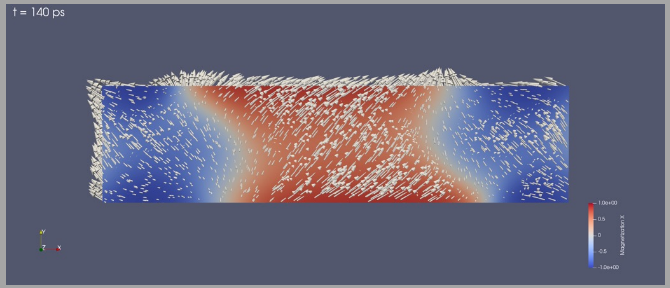
```
name = sp4_
scale = 1.e-9
mesh type = vtk
alpha = 0.02
initial state = fromfile_sp4_s-state.vtu
time step = 0.1 # demag refresh interval in ps
duration = 1000  # simulation time in ps
solver type = gpu

external field = 25.0 #  Hext in mT
    theta_H = 90 # polar angle of the field direction in degree
    phi_H = 170 # azimuthal angle
```

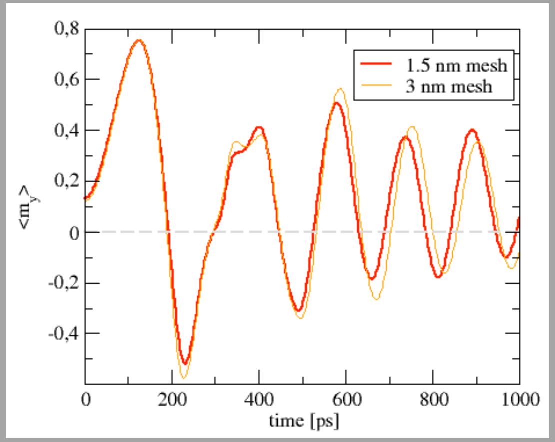
3. Run the simulation

```
hertel@euclide: ~/Docs/tetmag/example1
t[ps]: 2930.000 tot: 4883.169 de: 302.751 xc: 4580.418 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00101  0.00199 -0.00360
t[ps]: 2940.000 tot: 4883.166 de: 302.749 xc: 4580.417 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00102  0.00197 -0.00360
t[ps]: 2950.000 tot: 4883.164 de: 302.747 xc: 4580.417 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00104  0.00194 -0.00360
t[ps]: 2960.000 tot: 4883.161 de: 302.745 xc: 4580.416 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00105  0.00191 -0.00360
t[ps]: 2970.000 tot: 4883.159 de: 302.743 xc: 4580.416 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00106  0.00189 -0.00360
t[ps]: 2980.000 tot: 4883.156 de: 302.741 xc: 4580.415 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00108  0.00186 -0.00360
t[ps]: 2990.000 tot: 4883.154 de: 302.740 xc: 4580.415 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00109  0.00184 -0.00360
t[ps]: 3000.000 tot: 4883.152 de: 302.738 xc: 4580.414 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00110  0.00181 -0.00360
t[ps]: 3010.000 tot: 4883.150 de: 302.736 xc: 4580.414 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00111  0.00179 -0.00360
t[ps]: 3020.000 tot: 4883.148 de: 302.735 xc: 4580.413 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00112  0.00176 -0.00360
t[ps]: 3030.000 tot: 4883.146 de: 302.734 xc: 4580.413 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00113  0.00174 -0.00360
t[ps]: 3040.000 tot: 4883.145 de: 302.732 xc: 4580.412 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00114  0.00172 -0.00360
t[ps]: 3050.000 tot: 4883.143 de: 302.731 xc: 4580.412 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00115  0.00169 -0.00360
t[ps]: 3060.000 tot: 4883.141 de: 302.730 xc: 4580.412 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00116  0.00167 -0.00360
t[ps]: 3070.000 tot: 4883.140 de: 302.729 xc: 4580.411 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00116  0.00165 -0.00360
t[ps]: 3080.000 tot: 4883.138 de: 302.728 xc: 4580.411 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00117  0.00163 -0.00360
t[ps]: 3090.000 tot: 4883.137 de: 302.727 xc: 4580.410 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00118  0.00160 -0.00360
t[ps]: 3100.000 tot: 4883.136 de: 302.726 xc: 4580.410 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00118  0.00158 -0.00360
t[ps]: 3110.000 tot: 4883.134 de: 302.725 xc: 4580.410 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00119  0.00156 -0.00360
t[ps]: 3120.000 tot: 4883.133 de: 302.724 xc: 4580.409 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00120  0.00154 -0.00360
t[ps]: 3122.000 tot: 4883.133 de: 302.724 xc: 4580.409 un: 0.000 ze: -0.000 cb: 0.000 sf: 0.000 dm: 0.000       M:  0.00120  0.00154 -0.00360
Simulation finished.
simulation time: 00:05:51.505
hertel@euclide:~/Docs/tetmag/example1$
```

4. Analyze the results



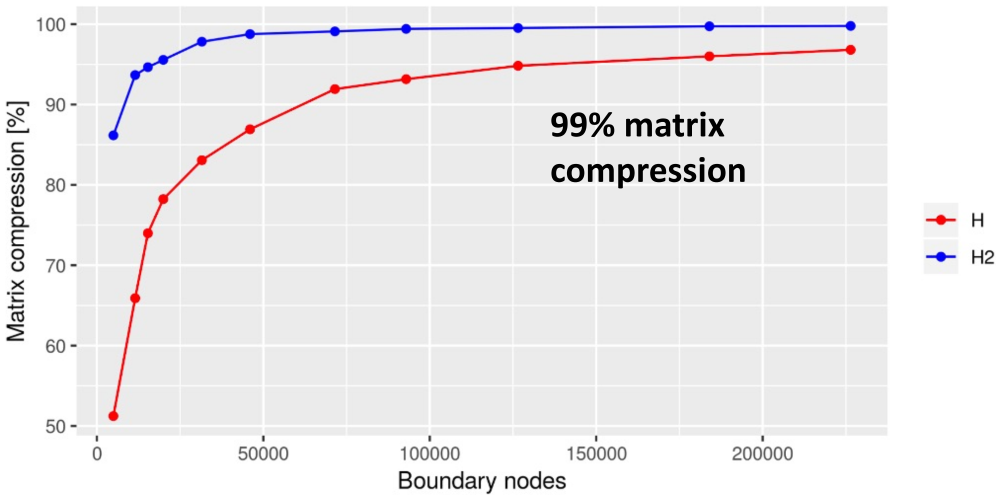

```
...
132.0000        19906.6614      18013.1318      2884.8823       0.0000  -991.3528       0.000
134.0000        19811.6267      18414.0172      3004.6501       0.0000  -1607.0406      0.000
136.0000        19712.4086      18811.0095      3126.6089       0.0000  -2225.2098      0.000
138.0000        19608.9898      19203.9153      3249.6787       0.0000  -2844.6042      0.000
140.0000        19501.3684      19592.6391      3372.7034       0.0000  -3463.9740      0.000
...
```



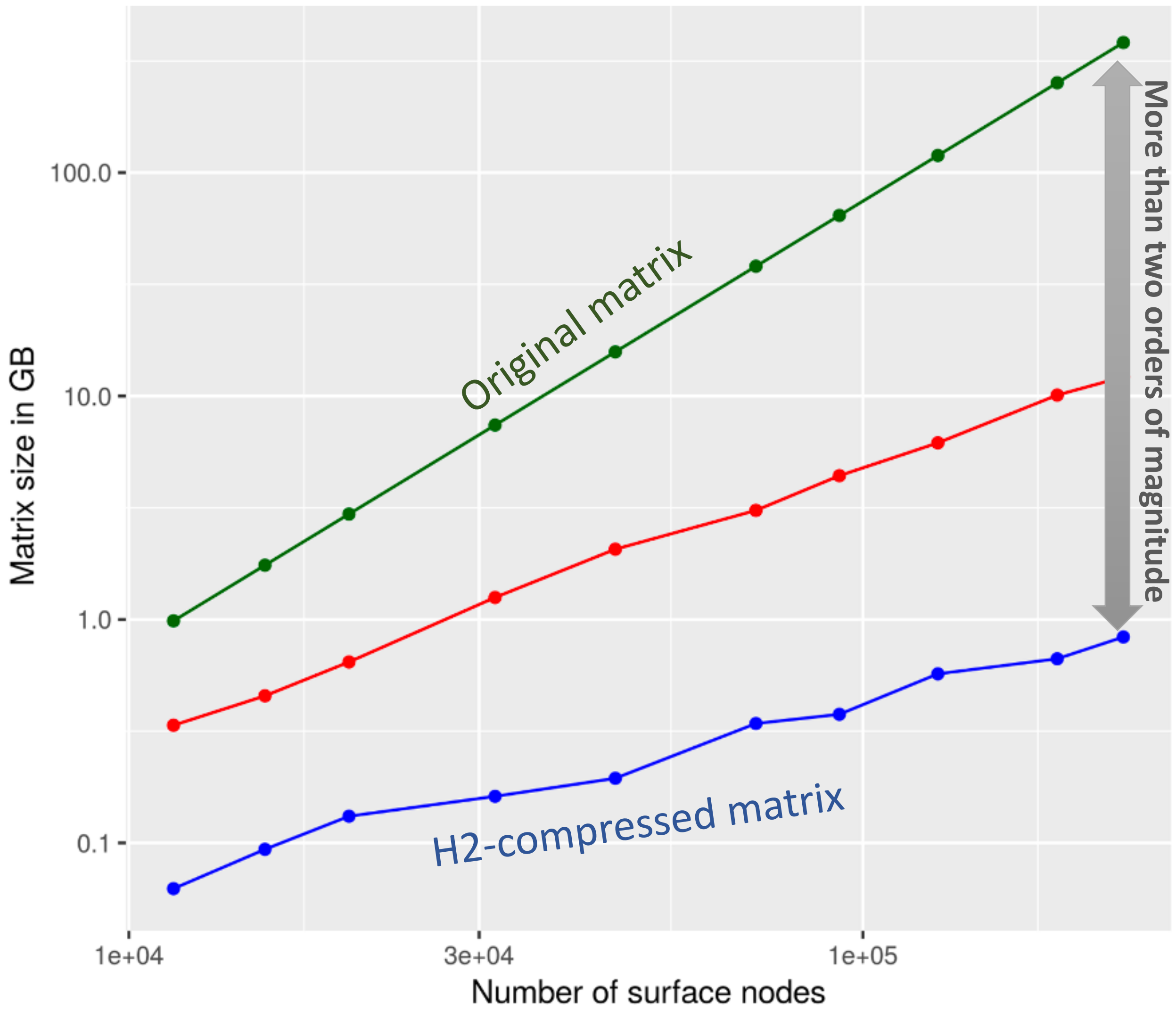
Importance of Advanced Mathematics and Numerics

Example: Calculation of dipolar magnetic field

Massive reduction of numerical costs
by using H2-type hierarchichal matrices



Converting a problem of
Complexity $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$



Efficient mathematical algorithms and numerical implementations can save large amounts of hardware resources and countless hours of CPU time

Hertel et al.,
J. Magn. Magn. Mater.
477, 118 (2019)

Part2: General remarks on scientific code development and best practices

Why publish your code?

- Service to the scientific community
- Reproducibility and transparence of published data
- Recognition of work done during (years of) code development
- Possible collaboration and code improvement by the community
- Removes necessity to protect the code against theft

Code publication encouraged by government

Specific funding for scientific code development?