面向应用的多物理场下微磁学仿真方法

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Email: wcyu@fudan.edu.cn

D. D. Stancil and A. Prabhakar, Spin waves (Springer, 2009).

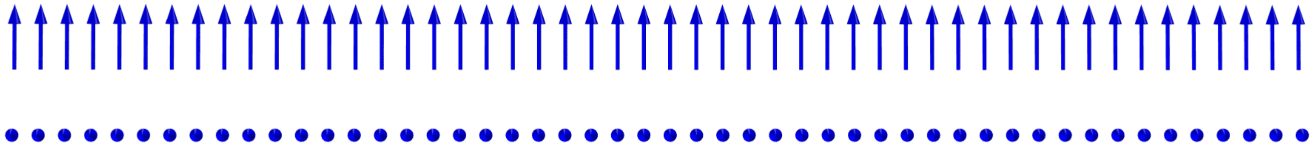
LLG(Landau-Lifshitz-Gilbert) 方程

$$\frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t} = -\gamma \mathbf{m}(\mathbf{r},t) \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m}(\mathbf{r},t) \times \frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t}$$

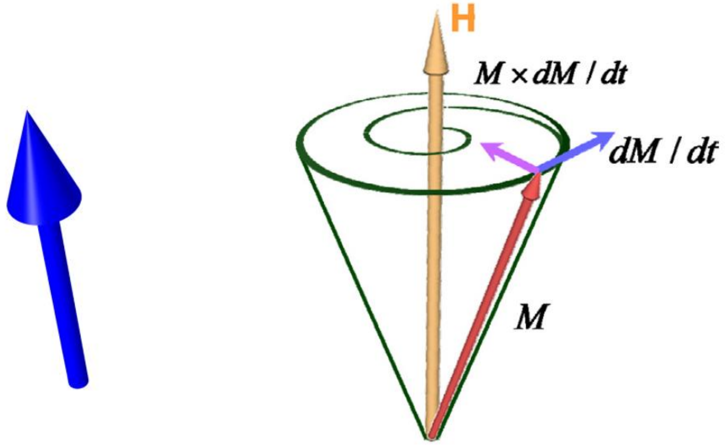
$\mathbf{H}_{\text{eff}}$ 有效场:

$A\nabla^2\mathbf{m}$	交换相互作用
$K\mathbf{m}\cdot\mathbf{e}$	磁晶各向异性
$\frac{1}{4\pi}\int\left(\frac{3\mathbf{r}(\mathbf{m}\cdot\mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3}\right)d\mathbf{r}$	磁偶极相互作用
$-D\nabla\times\mathbf{m}$	DM相互作用
···	等等

自旋波（磁子）

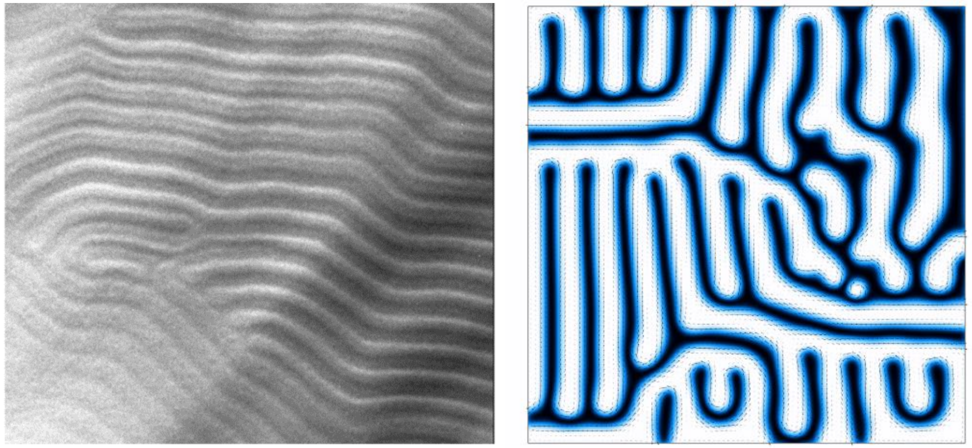


磁矩进动



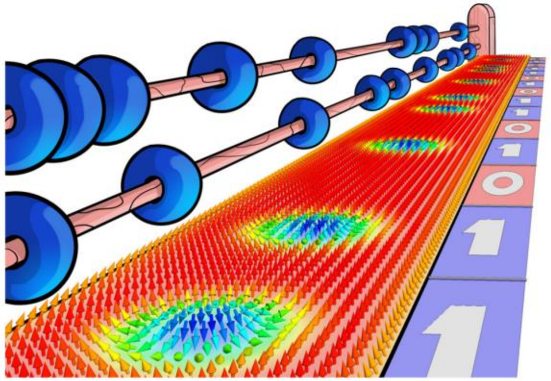
S. K. Kim, J. Phys. D: Appl. Phys. 43 (2010)

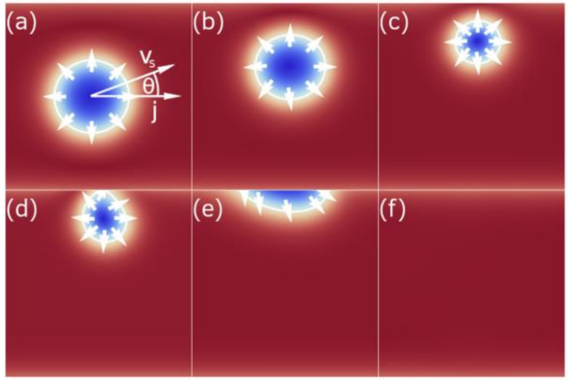
磁结构

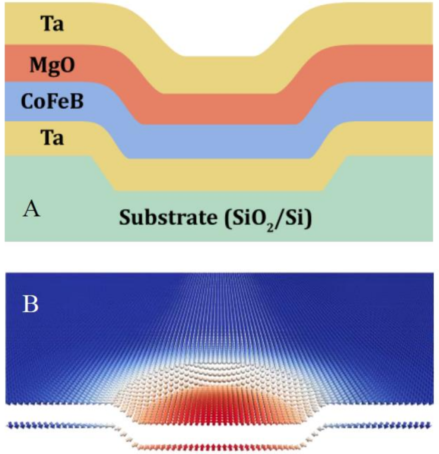


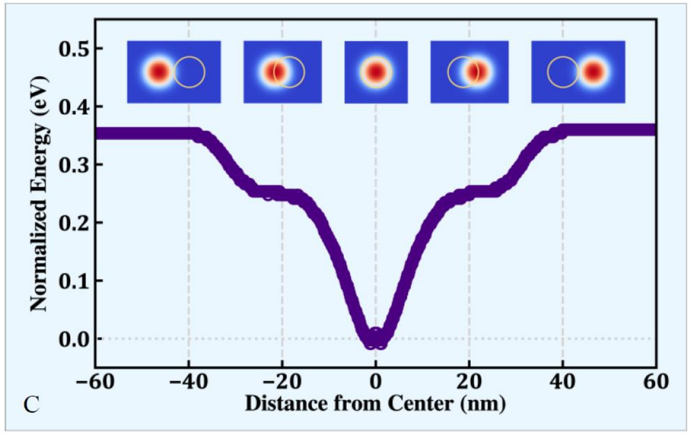
PNAS, 2012, 109(23): 8856-8860.

磁性斯格明子（magnetic skyrmions）



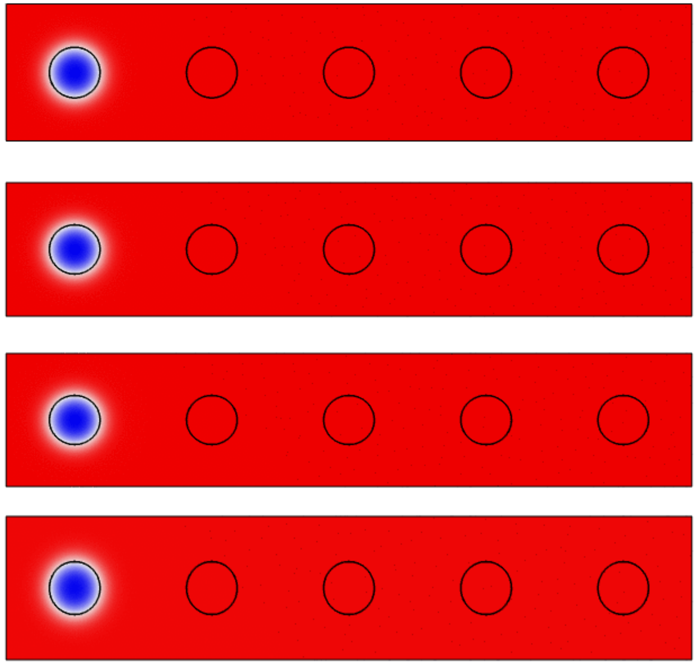




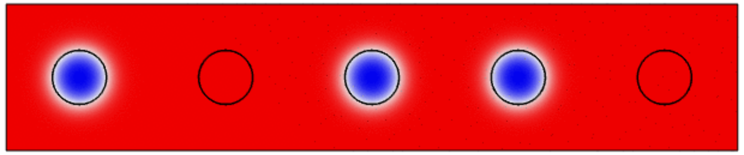


J. Appl. Phys. 124, 240901 (2018)

自旋轨道矩： $\boldsymbol{\tau} = -\gamma \frac{\hbar \theta_{\mathrm{sh}} j_{\mathrm{HM}}}{2\mu_0 e M_{\mathrm{s}} d} \boldsymbol{m} \times (\boldsymbol{m} \times \boldsymbol{p})$



“1011” :



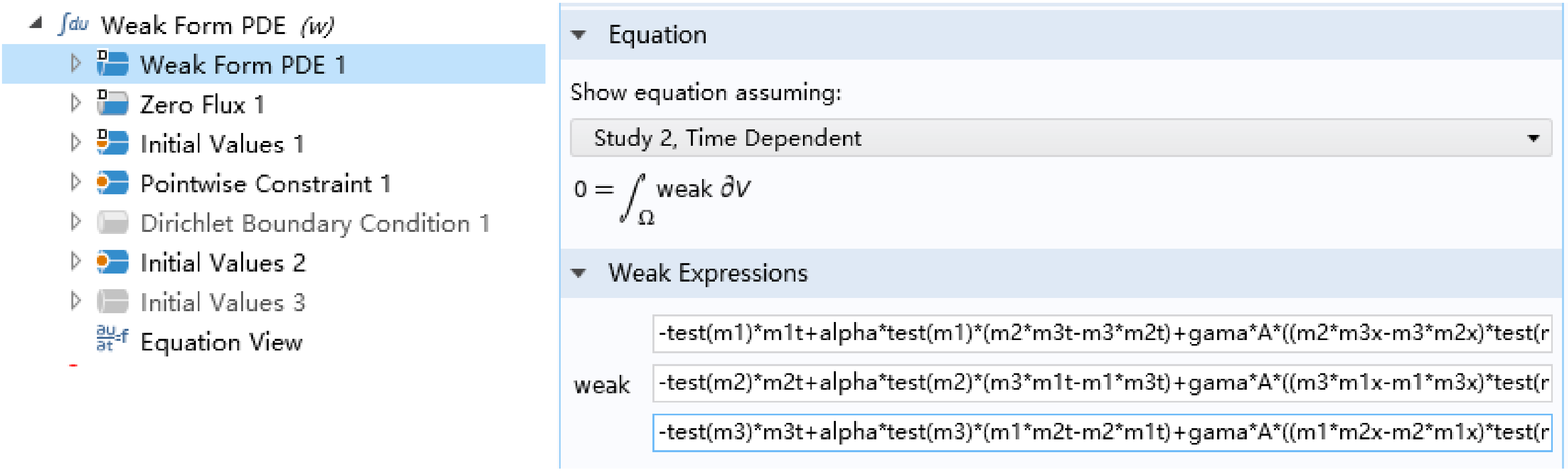
Le Zhao, Chensong Hua, Chengkun Song, Weichao Yu and Wanjun Jiang. **Science Bulletin** 69, 2370-2378 (2024)

LLG(Landau-Lifshitz-Gilbert) 方程

$$\frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t} = -\gamma \mathbf{m}(\mathbf{r},t) \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m}(\mathbf{r},t) \times \frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t}$$

系数型PDE无法定义

需转换成弱形式



微磁学仿真软件

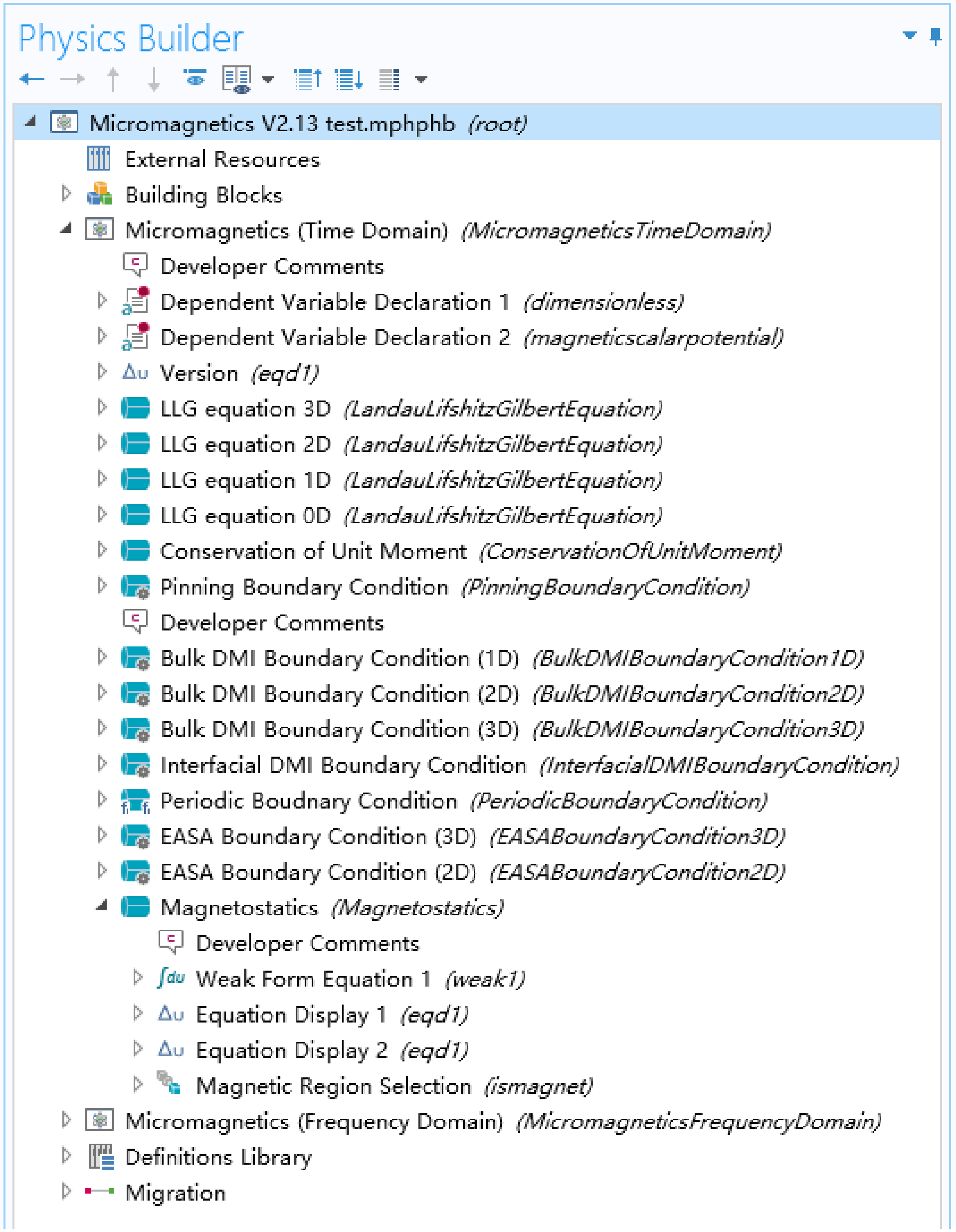
OOMMF

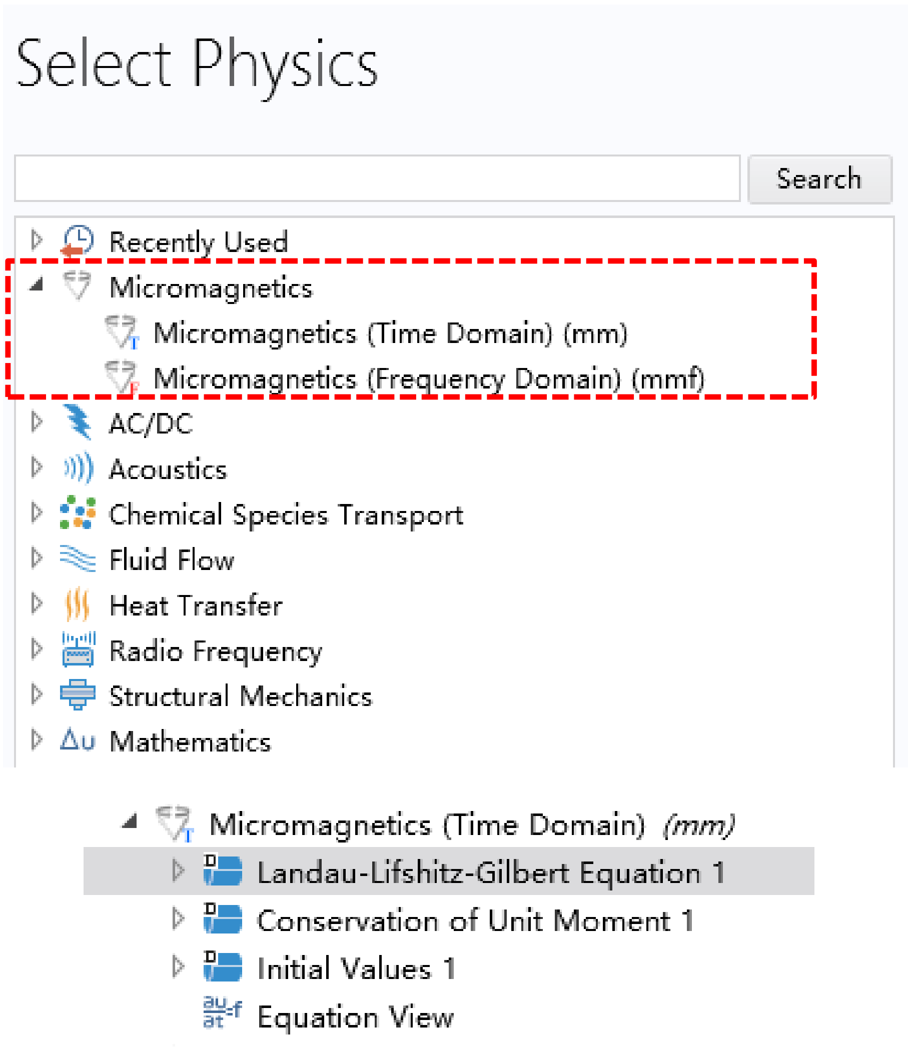
MuMax3

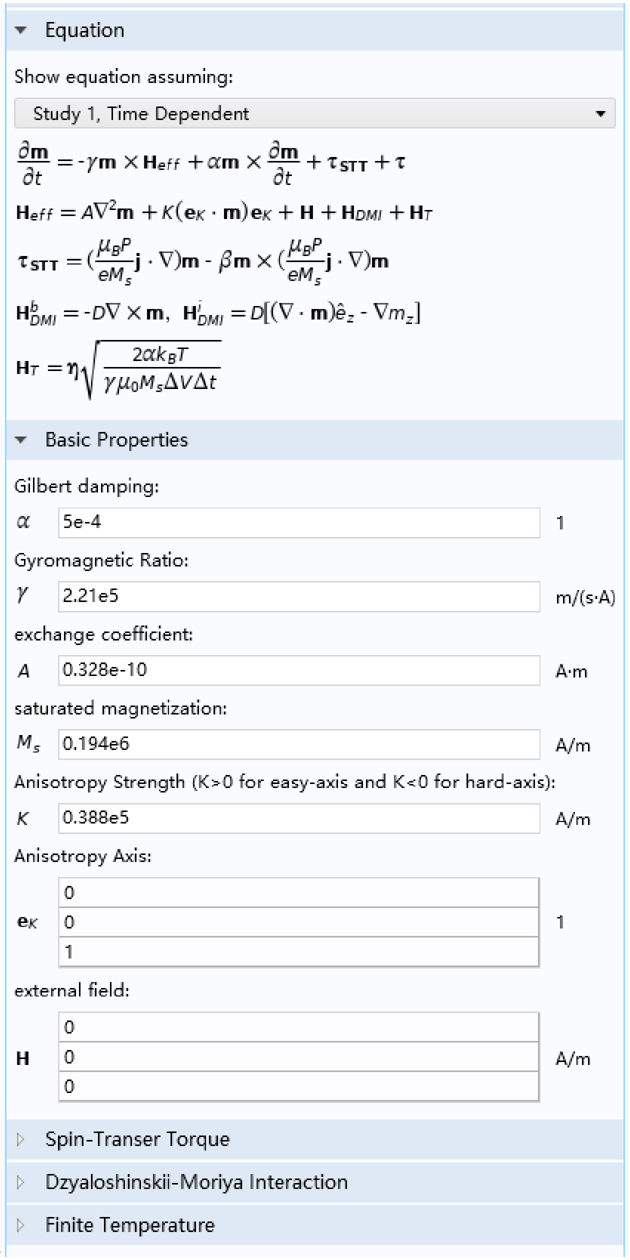
Ubermag

微磁学仿真模块

https://cn.comsol.com/blogs/micromagnetic-simulation-with-comsol-multiphysics/







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封装完后可分发给其他用户使用

Application Exchange

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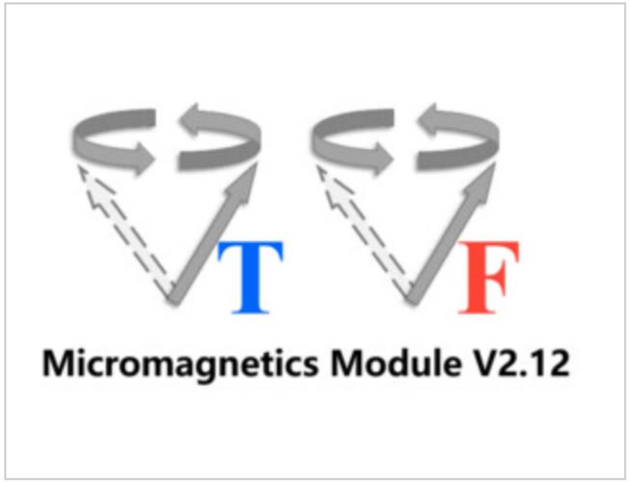
Micromagnetics Module for COMSOL Multiphysics

伟超 余, 复旦大学
Email: wcyu@fudan.edu.cn

Micromagnetics Module has been updated to V2.12. Please note that the new module is not compatible with the mph files created by versions before V2.0.

The dynamics of magnetization in magnets are described by micromagnetic theory, governed by the Landu–Lifshitz–Gilbert equations. We built a customized "Micromagnetics Module" using the Physics Builder in the COMSOL Multiphysics® software, which can be used to perform micromagnetic simulations within the framework of the COMSOL® software. This Micromagnetics Module can be coupled straightforwardly to other add-on modules to perform multiphysics micromagnetic simulations, such as magneto-dipolar coupling, magnetoelastic coupling, magnet-thermal coupling, and more. The module package, along with a user's guide, is available for download.

Questions and comments are encouraged to be left here.



Filename	Size
Micromagnetics...Guide V2.12.pdf	13.6 MB
Micromagnetics Module.jar	1,009 KB
Download all files (Zip-archive)	~ 11.7 MB

时域+频域

微磁学仿真软件

OOMMF

MuMax3

Ubermag

只有时域

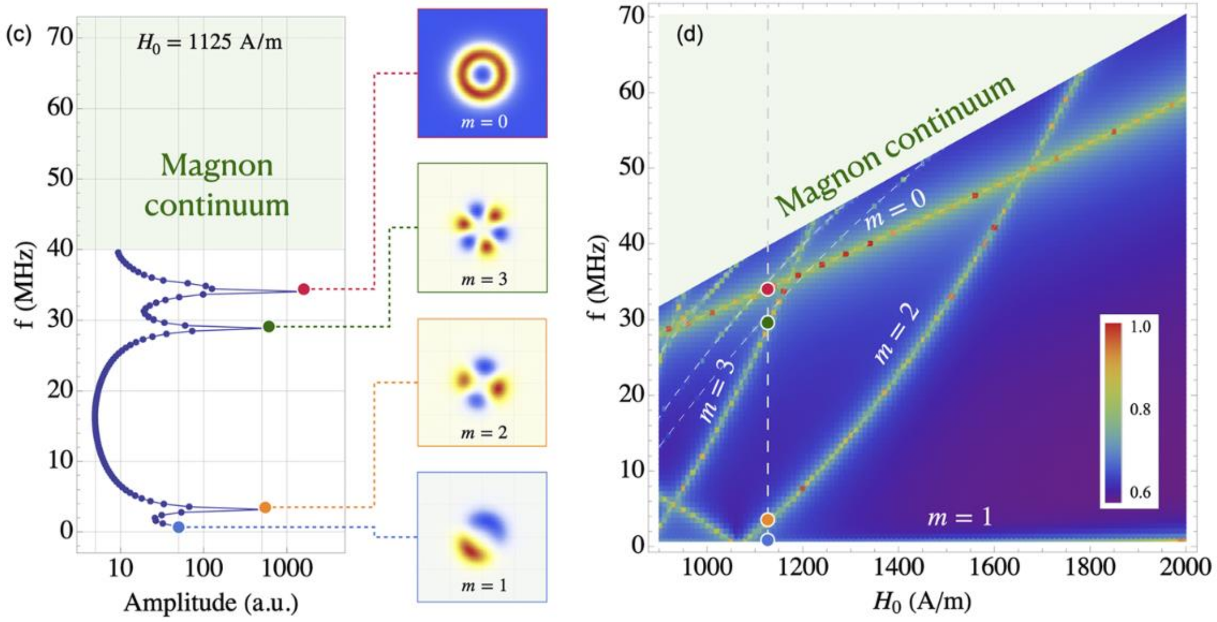
Jiabin Zhang, Weichao Yu†, Xiheng Chen and Jiang Xiao†, AIP Advances 13, 055108 (2023)

LLG方程（频域）$i\omega\delta\mathbf{m} = -\gamma\mathbf{m}_0 \times \delta\mathbf{h}^{\rm eff} - \gamma\delta\mathbf{m} \times \mathbf{h}_0^{\rm eff} + i\omega\alpha\mathbf{m}_0 \times \delta\mathbf{m}$

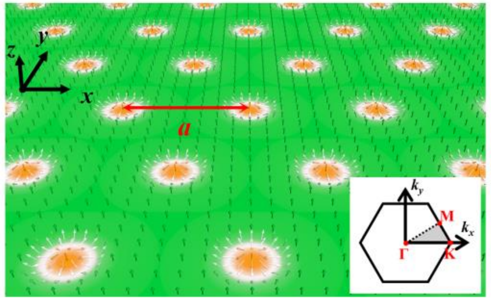
傅里叶变换（时域→频域） $\mathbf{m} = \mathbf{m}_0 + \delta\mathbf{m}e^{i\omega t}$

傅里叶变换（空间→倒空间） $\delta\mathbf{m}_{\rm dst} = \delta\mathbf{m}_{\rm src}e^{-i\mathbf{k}_F\cdot(\mathbf{r}_{\rm dst}-\mathbf{r}_{\rm src})}$

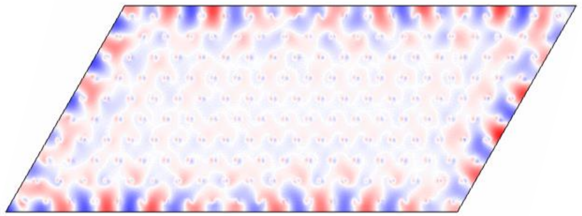
基于COMSOL的微磁学仿真模块（频域）



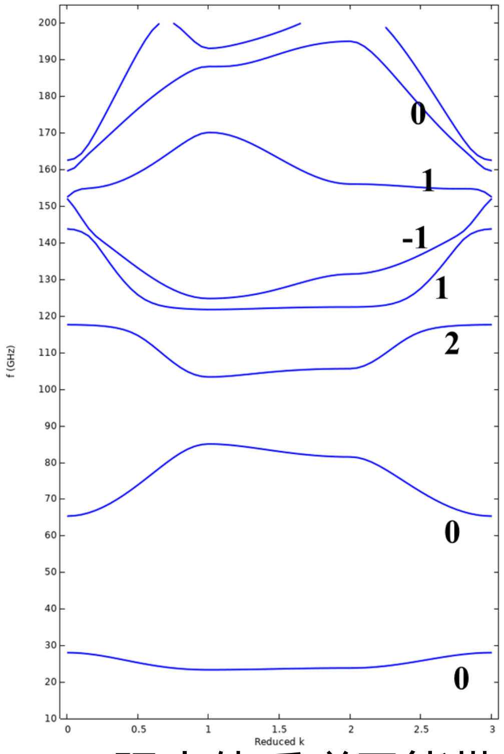
单个斯格明子激发谱



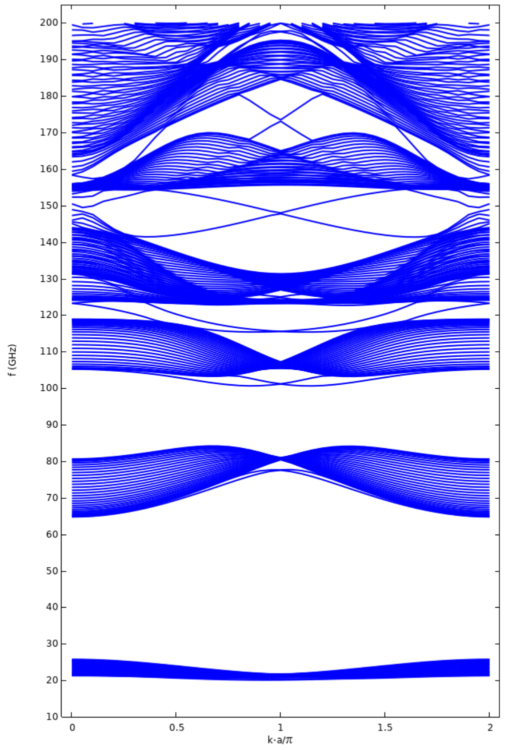
J. Appl. Phys. 130, 153901 (2021)



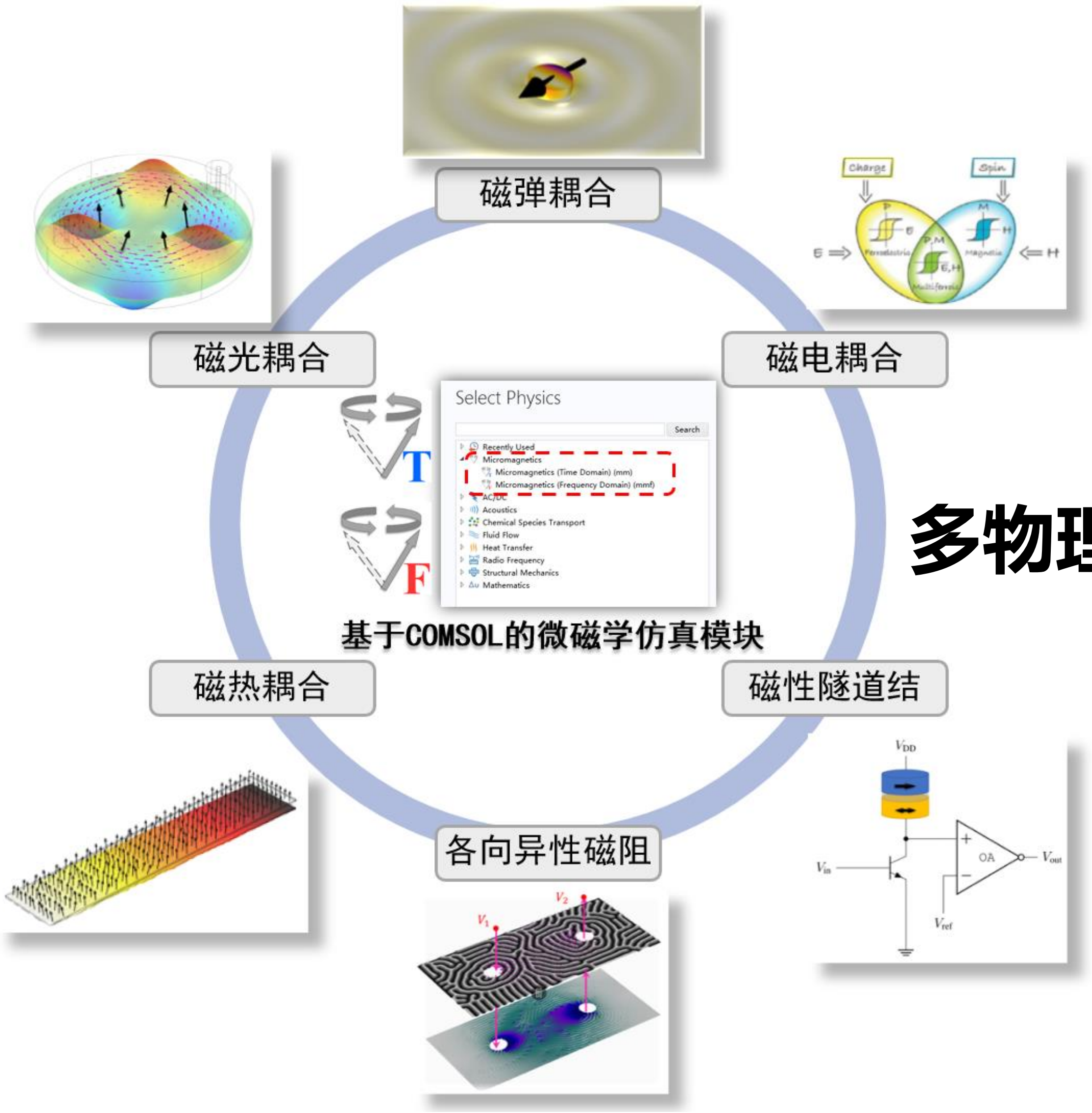
拓扑边界态



无限大体系磁子能带



受限体系磁子能带



多物理场耦合

麦克斯韦方程

$$\nabla\times(\nabla\times\mathbf{h})-(i\sigma\omega-\epsilon\omega^{2})\mathbf{b}=0$$

弹性波方程

$$\rho\frac{\partial^{2}\mathbf{u}}{\partial t^{2}}=\mu\nabla^{2}\mathbf{u}+(\lambda+\mu)\nabla(\nabla\cdot\mathbf{u})$$

欧姆定律

$$\mathbf{j}(\mathbf{r})=\Sigma[\mathbf{m}(\mathbf{r})]\cdot\mathbf{E}(\mathbf{r})$$

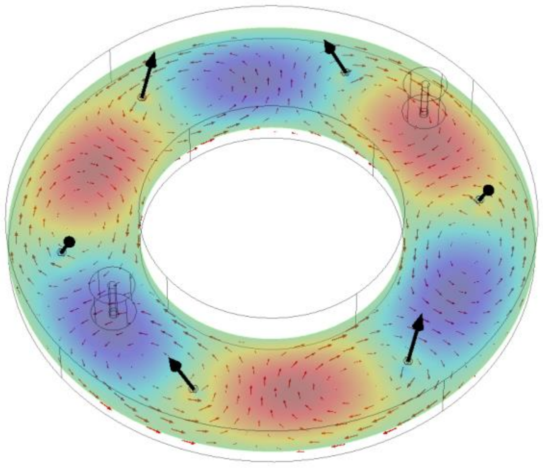
铁电LKT方程

$$\alpha_0\frac{\partial^2 P}{\partial t^2}+\gamma_\nu\frac{\partial P}{\partial t}+\alpha_1 P+\alpha_2 P^3-\kappa\nabla^2 P=E$$

热传导方程

$$\rho C_p\frac{\partial T}{\partial t}+\rho C_p\mathbf{v}\cdot\nabla T-\kappa\nabla^{2}T=Q$$

……



PHYSICAL REVIEW B 102, 064416 (2020)

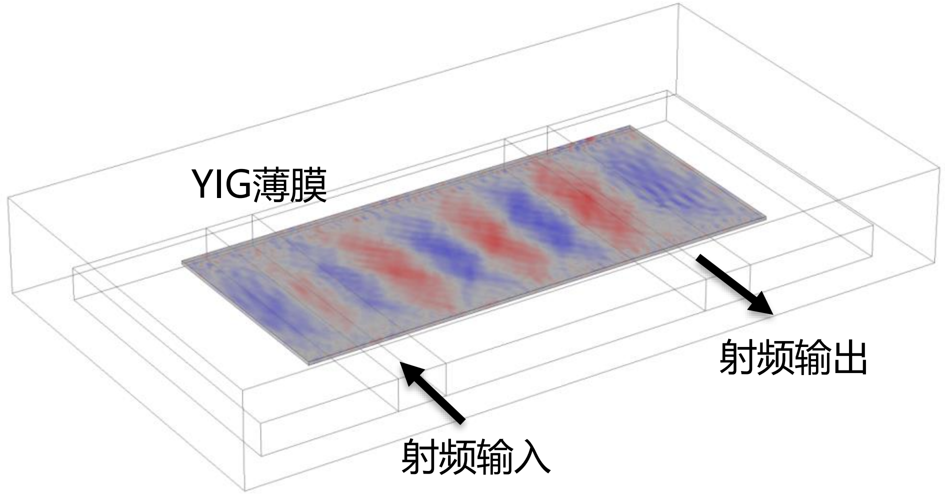
麦克斯韦方程

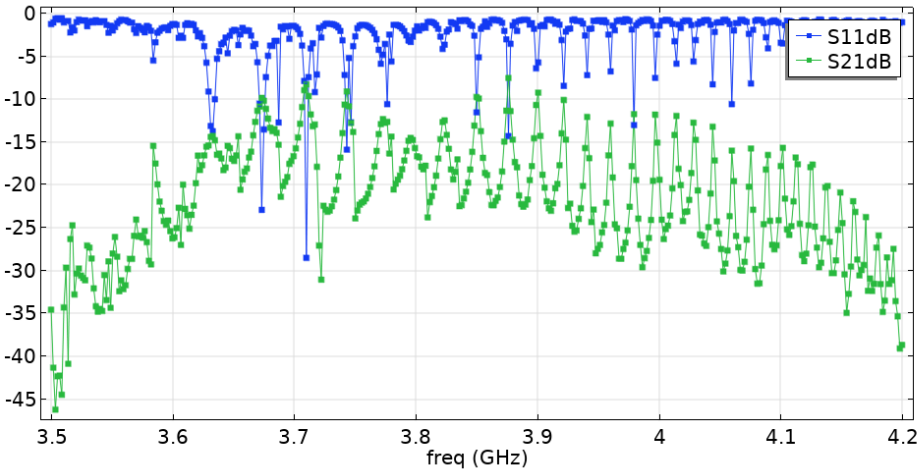
$$\nabla \times (\nabla \times \mathbf{h}) - (i\sigma\omega - \epsilon\omega^2)\mathbf{b} = 0$$

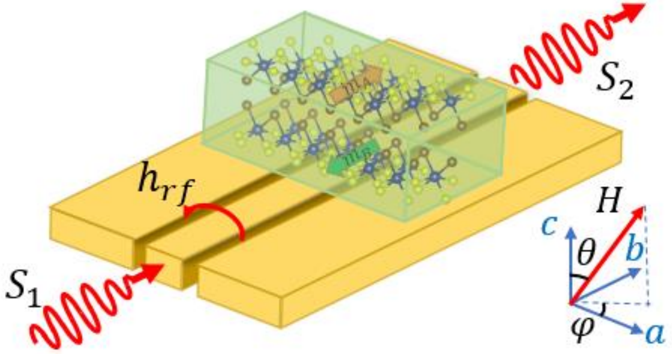
塞曼相互作用

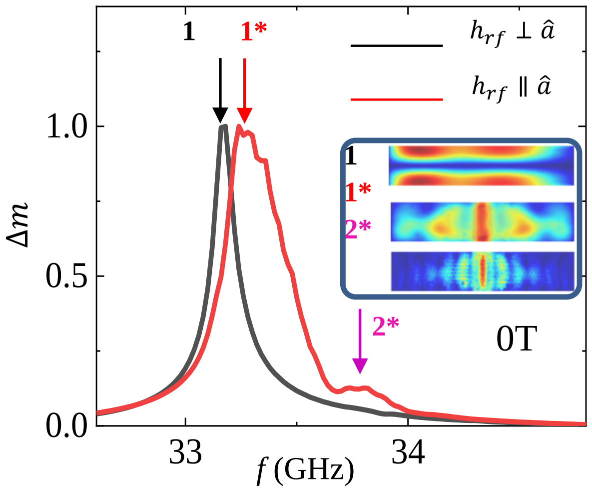
$$\mathcal{H}_{\mathrm{Zeeman}} = -\mu_0 M_s \mathbf{m} \cdot \mathbf{h}$$

频率选择限幅器(FSL)透射反射谱





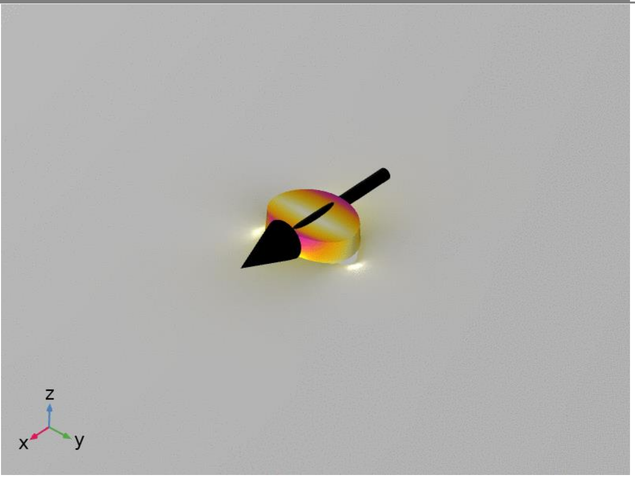




CrSBr反铁磁共振

Hongyue Xu, ... Weichao Yu and Yizheng Wu. unpublished

C. Kittel, Phys. Rev. 110, 836 (1958)



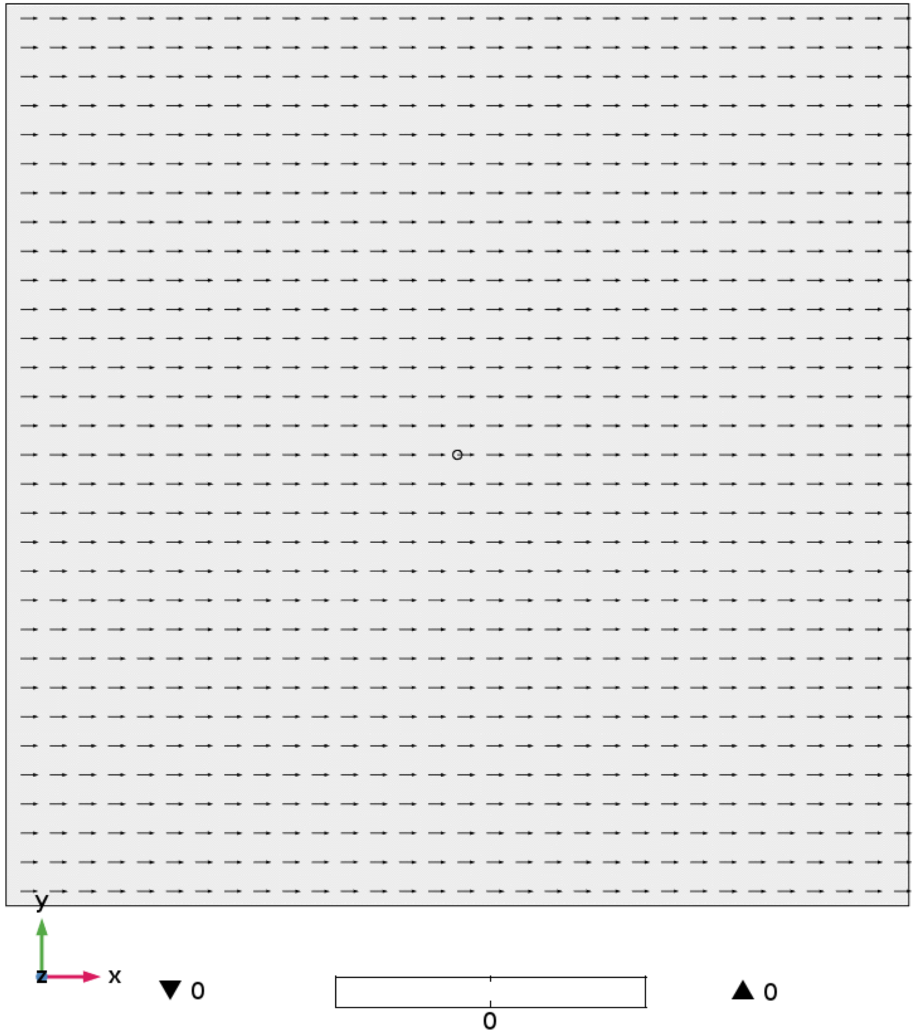
弹性波运动方程

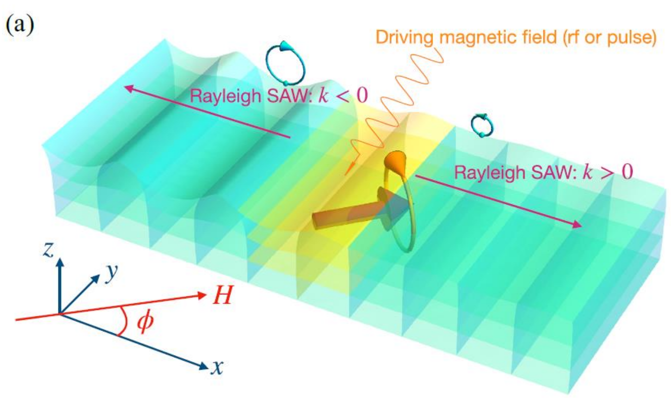
$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \mu \nabla^2 \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u})$$

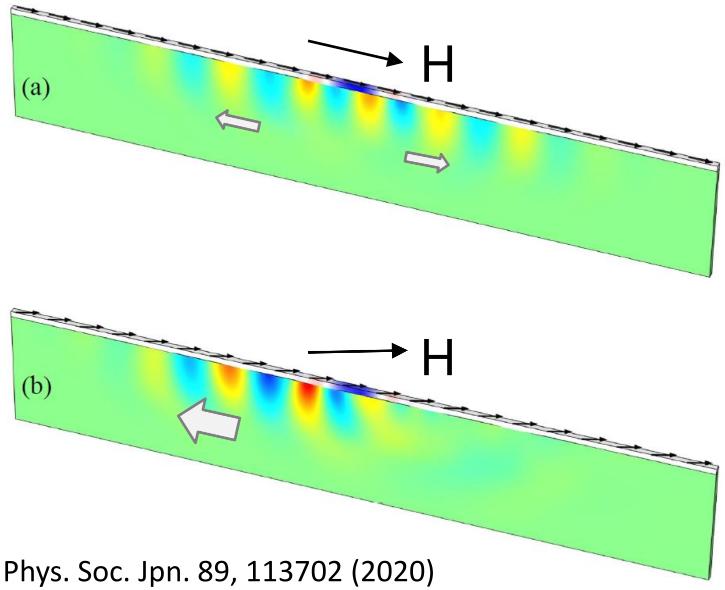
磁弹相互作用

$$H_{\mathrm{MEC}} = b_1 \sum_i m_i^2 S_{ii} + b_2 \sum_{i \neq j} m_i m_j S_{ij}$$

磁子-声子极化激元 (magnon polaron)







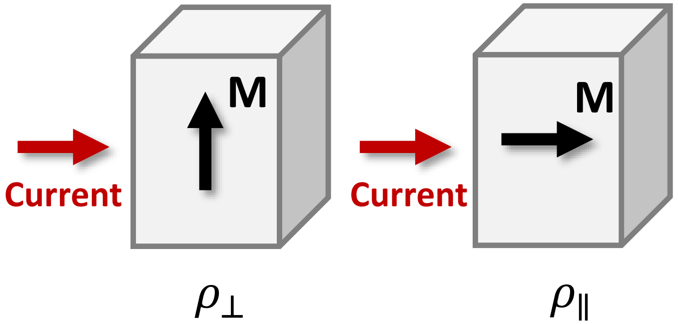
Yamamoto, **Yu**, et al. J. Phys. Soc. Jpn. 89, 113702 (2020)

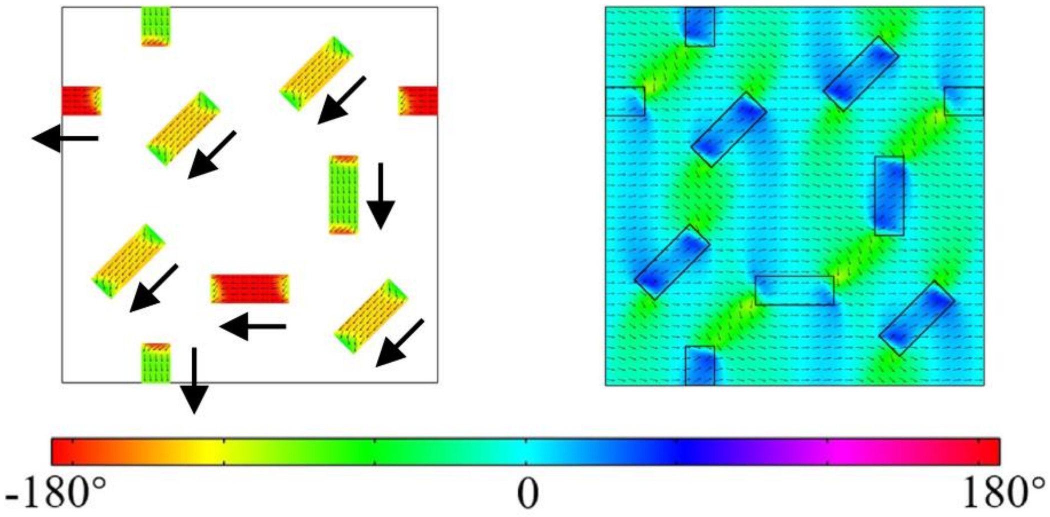
非互易声波泵浦

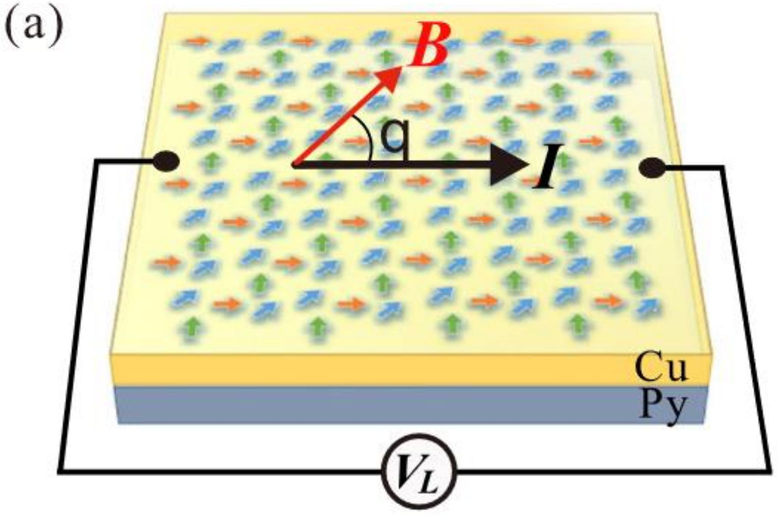
各向异性磁电阻 (AMR)

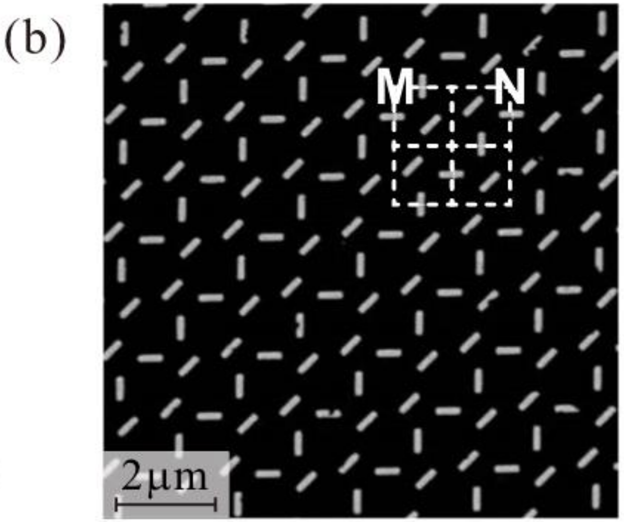
$$\rho = \rho_{\perp} + (\rho_{\parallel} - \rho_{\perp}) \cos^2 \theta$$

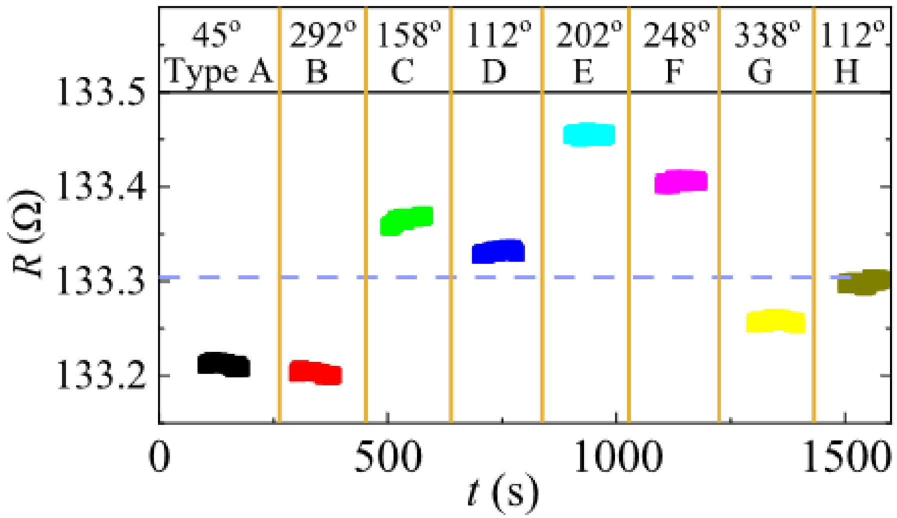
欧姆定律







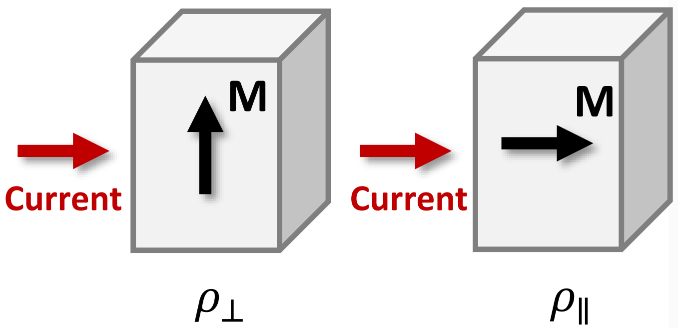




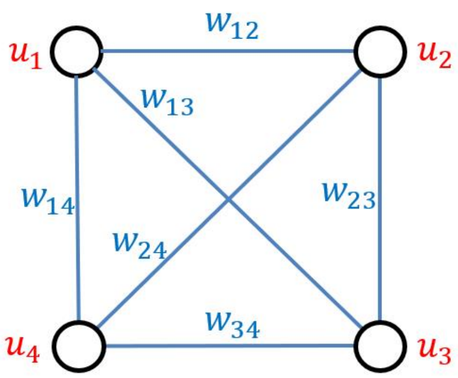
人工自旋冰（artificial spin ice）

各向异性磁电阻 (AMR)

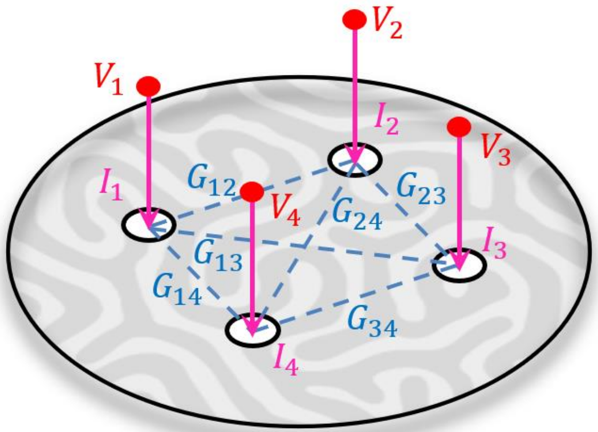
$$\rho = \rho_\perp + (\rho_\parallel - \rho_\perp)\cos^2\theta$$



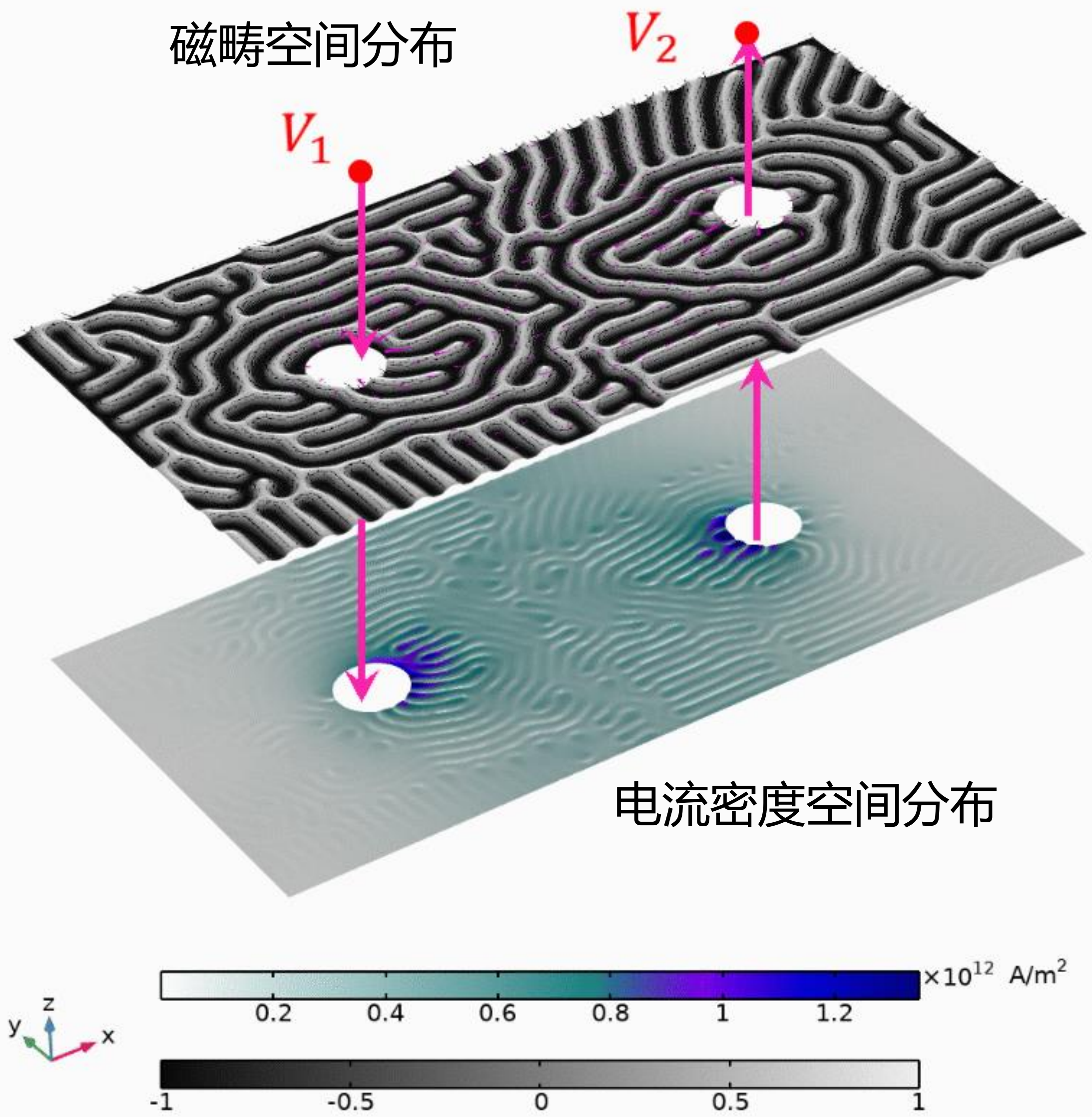
欧姆定律 $\mathbf{j}(\mathbf{r}) = \Sigma[\mathbf{m}(\mathbf{r})]\cdot\mathbf{E}(\mathbf{r})$



$u_i' = \Sigma_{j\neq i} w_{ij} u_j$



$I_i = \Sigma_j G_{ij} V_j$



具备自主学习和联想记忆能力的的磁性Hopfield网络

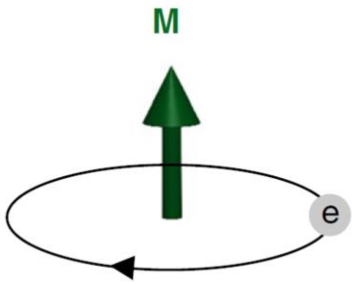
The Nobel Prize in Physics 2024 John Hopfield

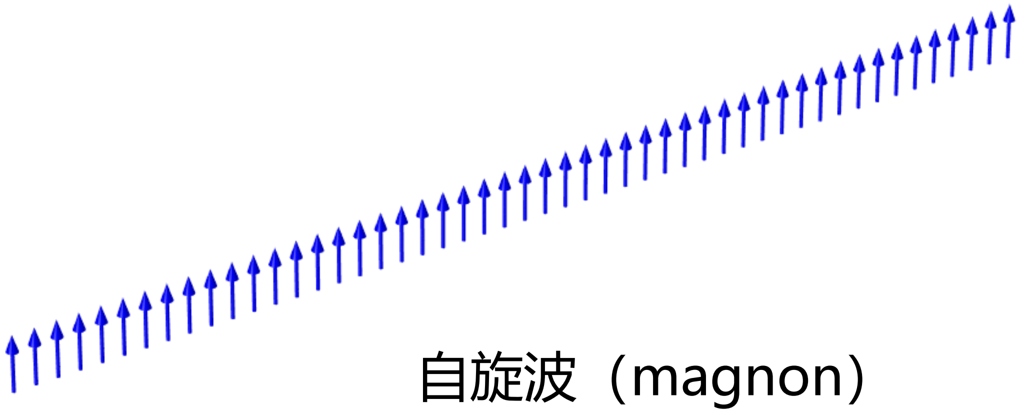
微磁学仿真

LLG(Landau-Lifshitz-Gilbert) 方程

$$\frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t} = -\gamma \mathbf{m}(\mathbf{r},t) \times \mathbf{H}_{\mathbf{eff}} + \alpha \mathbf{m}(\mathbf{r},t) \times \frac{\partial \mathbf{m}(\mathbf{r},t)}{\partial t}$$

自发磁化 $\boldsymbol{M} = M_S \boldsymbol{m}$





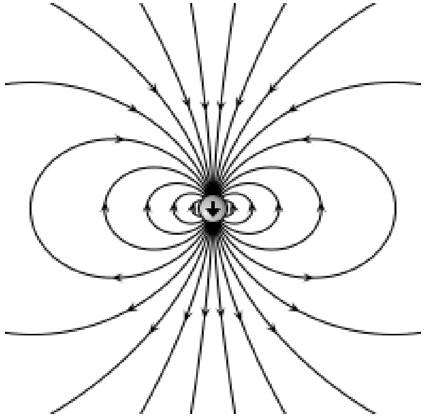
自旋波（magnon）

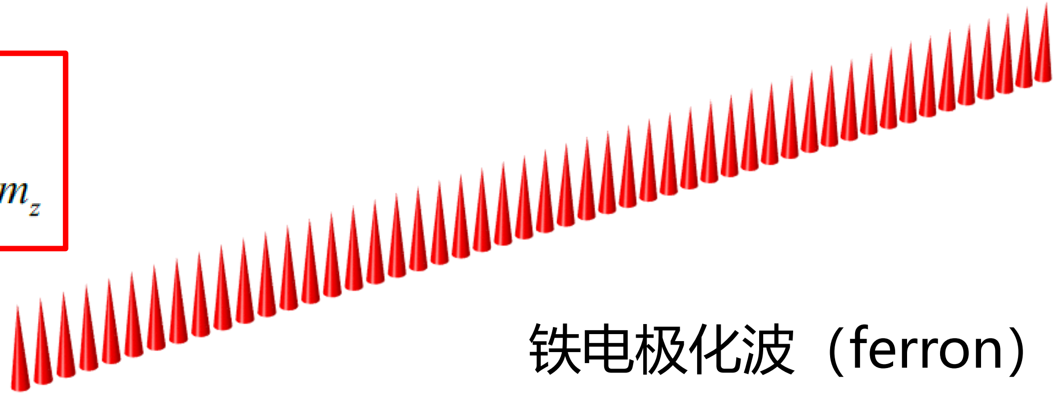
铁电相场模拟

LKT(Landau-Khalatnikov-Tani) 方程

$$\alpha_0 \frac{\partial^2 P}{\partial t^2} + \gamma_\nu \frac{\partial P}{\partial t} + \alpha_1 P + \alpha_2 P^3 - \kappa \nabla^2 P = E$$

自发极化 $P_0 = \sqrt{-\frac{\alpha_1}{\alpha_2}}$





铁电极化波（ferron）

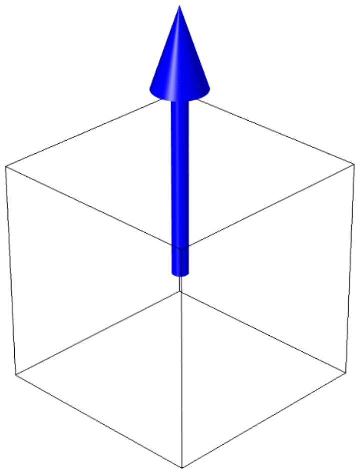
磁电耦合

$$F_{\mathrm{ME}} = -gPM_s m_z$$

W.F. Brown, Journal of Applied Physics, 1963, 34(4): 1319-20.

有限温度下的热扰动随机场

$$H_T(\mathbf{r},t)=\boldsymbol{\eta}\sqrt{\frac{2k_B T\alpha}{\gamma V\mu_0 M_s \Delta V \Delta t}}$$

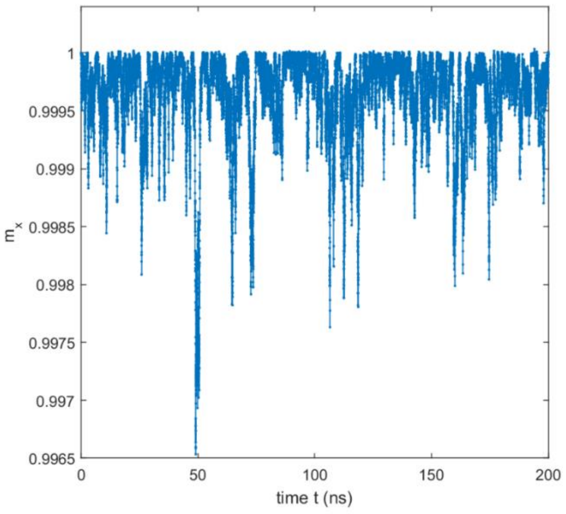


体系状态服从玻尔兹曼分布

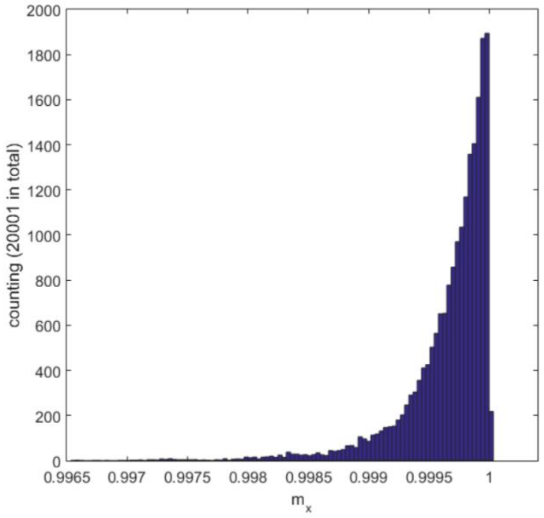
$$P(E)\propto e^{-\beta E}$$

热传导方程 $$\rho C_p\frac{\partial T}{\partial t}+\rho C_p\mathbf{v}\cdot\nabla T-\kappa\nabla^2 T=Q$$

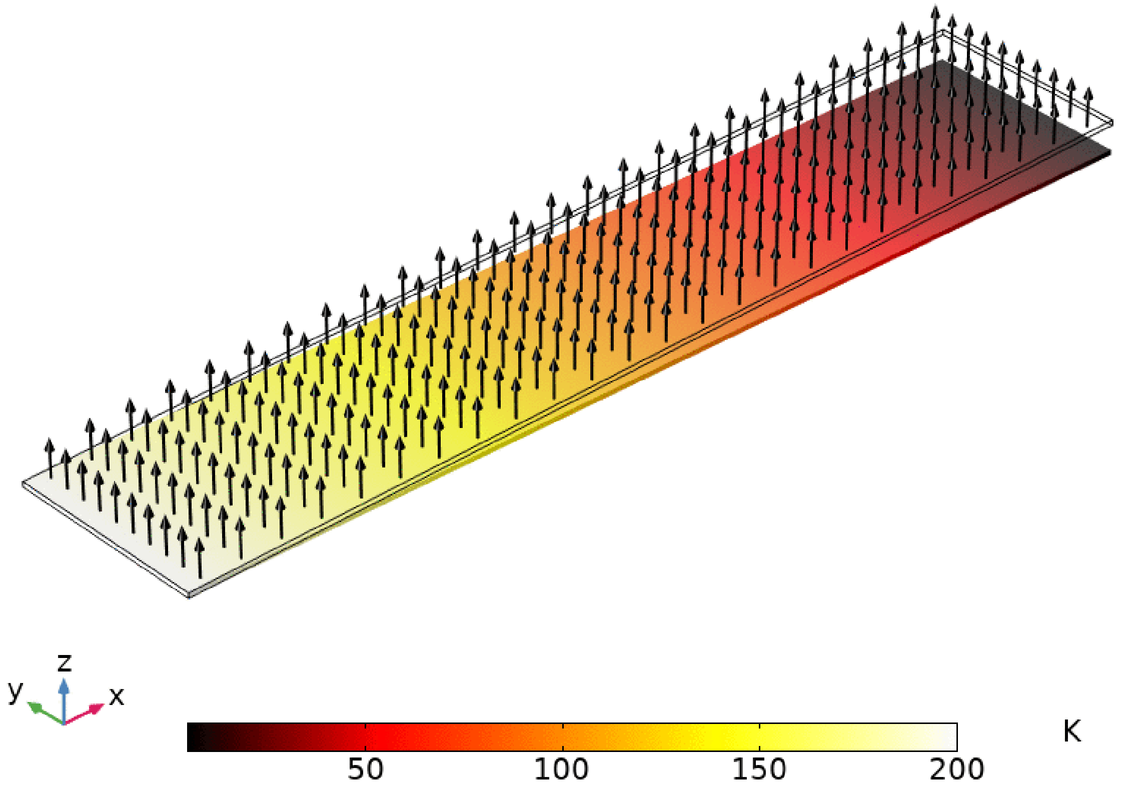
磁阻尼致热耗散 $$Q=\frac{\alpha M_s}{\gamma}\left(\frac{\partial\mathbf{m}}{\partial t}\right)^2$$



(a) temporal distribution of m_x

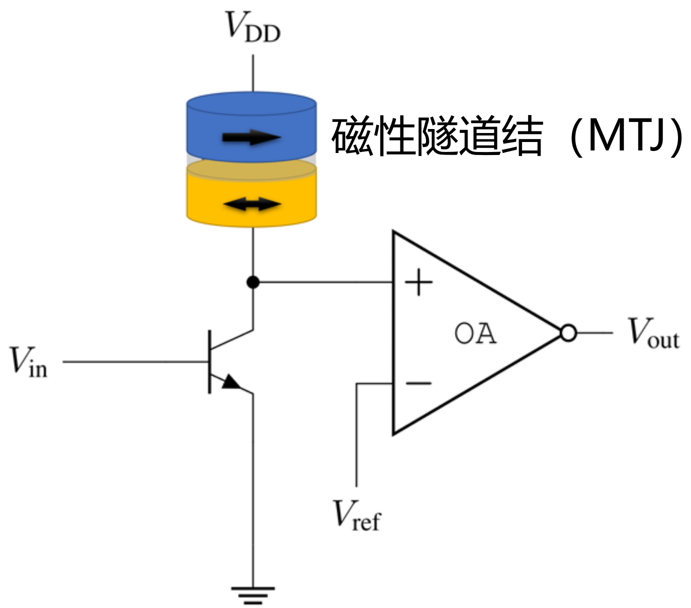


(b) histrogram of m_x



概率计算

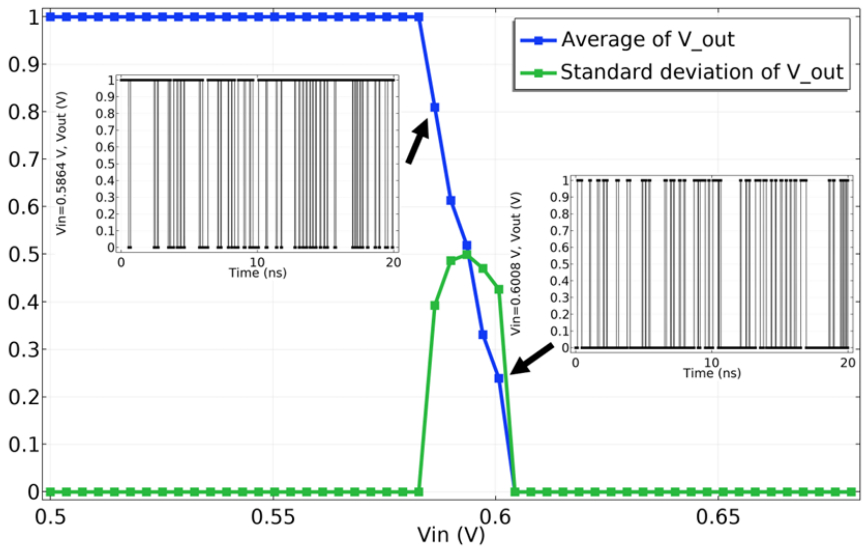
K. Y. Camsari, S. Salahuddin, and S. Datta,, IEEE Electron Device Letters 38, 1767 (2017)

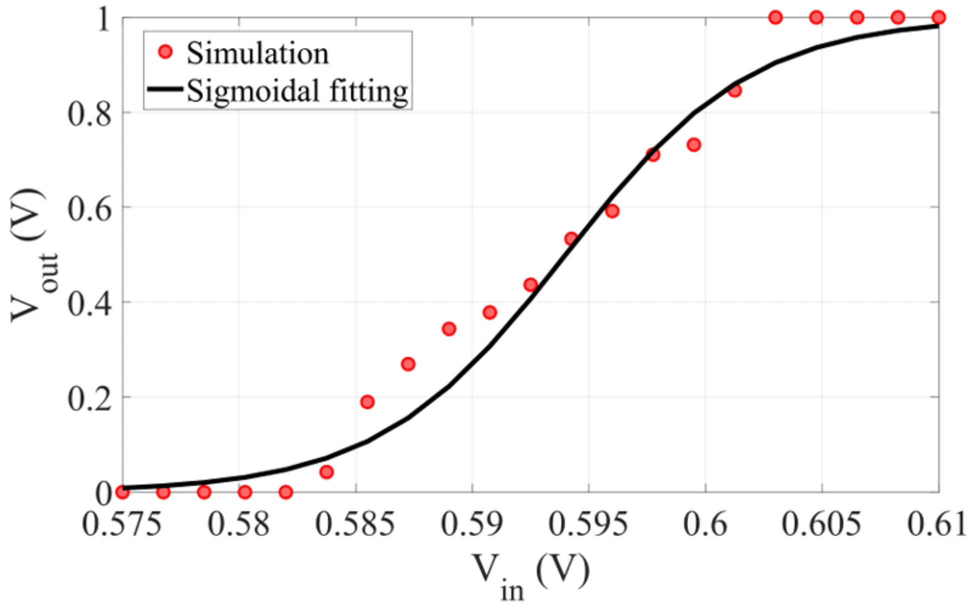


零维（0D）LLG方程 $$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H}_{\rm eff} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t} + \frac{\mu_{\rm B} P}{e M_{\rm s} V} \mathbf{m} \times \mathbf{I} \times \mathbf{m} - \beta \frac{\mu_{\rm B} P}{e M_{\rm s} V} \mathbf{I} \times \mathbf{m}$$

有限温下有效场 $$\mathbf{H}_{\rm eff} = -M_{\rm s} \mathbf{m} \cdot \hat{\mathbf{z}} + \boldsymbol{\eta} \sqrt{\frac{2\alpha k_{\rm B} T}{\gamma \mu_0 M_s V \Delta t}}$$

等效电阻 $$G(t) = G_0 \left[1 + \frac{\rm TMR}{2 + {\rm TMR}} m_x(t) \right]$$





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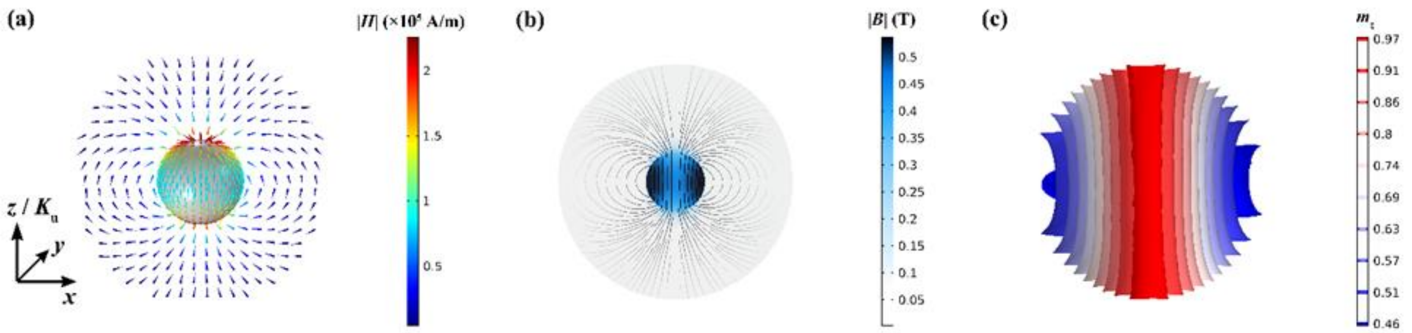
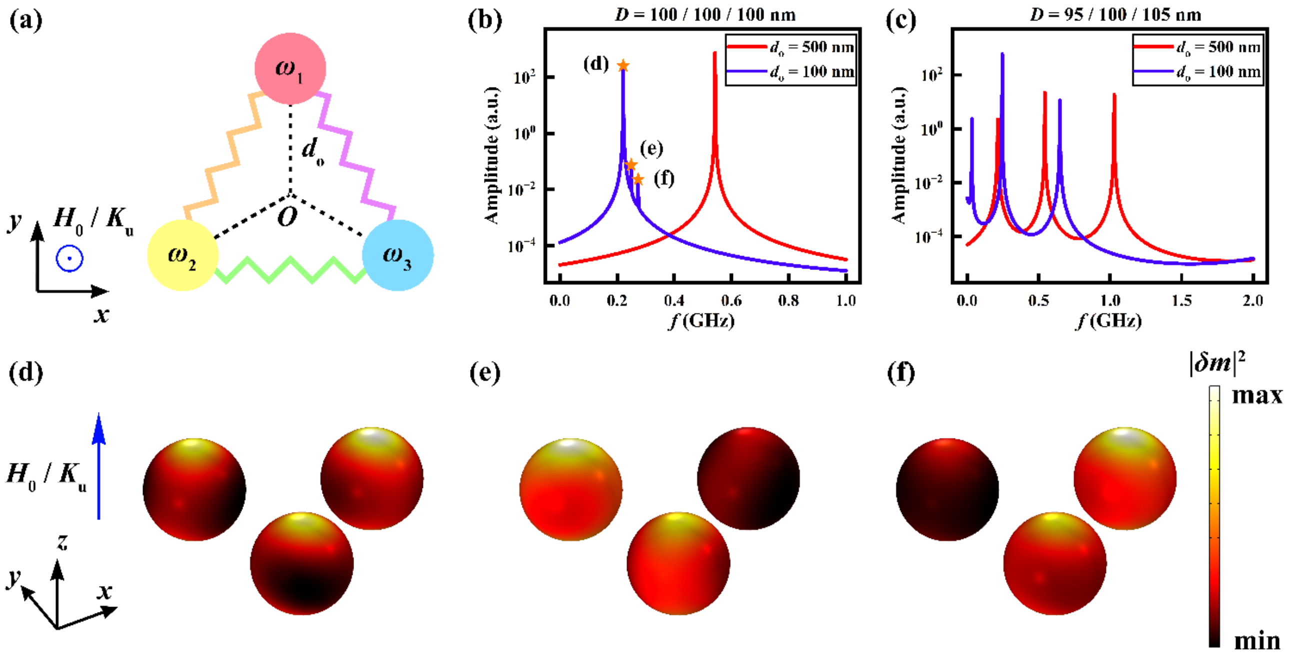
静态结构



动态响应



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Chapter 2

Micromagnetic simulation tools: OOMMF, Mumax^3, and COMSOL Multiphysics

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2.1 Introduction

Magnetic nanoparticles (MNPs) are mesoscale objects in nanometer orders (Wu et al., 2019). It's too tedious to apply the quantum treatment on every single spin embedded in the huge ensemble, meanwhile, it's not sufficient to treat the magnetizations in a whole particle as a single macro-spin. A better solution is to apply the theory called micromagnetics, which deals with magnetic behaviors at submicrometer scales. Such a scale is able to resolve magnetic structures such as domain walls and vortices while ignoring the atomic structure of specific materials. Hence, micromagnetics is a theory in the continuum, assuming the conservation of the magnetization magnitude. Even with the approximate treatment, there are still large degrees of freedom that cannot be solved by hand, and the technique to solve micromagnetic problems in a numerical way is called *micromagnetic simulation*, which has been successfully applied to verify experimental observation (Kim, 2010) as well as predict new phenomena (Leliaert & Mulkers, 2019). In this chapter, we will introduce the application of micromagnetic simulation in studying the static and dynamic properties of MNPs.

2.2 Theoretical background of micromagnetic simulation

2.2.1 Landau–Lifshitz–Gilbert equation

The governing equation of micromagnetism is the Landau–Lifshitz–Gilbert (LLG) equation (Bar'yakhtar & Ivanov, 2015; Gurevich & Melkov, 1996; Tserkovnyak et al., 2005):

$$\frac{\partial \mathbf{m}}{\partial t} = -\gamma \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t}, \tag{2.1}$$

Magnetic Nanoparticles in Nanomedicine. https://doi.org/10.1016/B978-0-443-21668-8.00002-X
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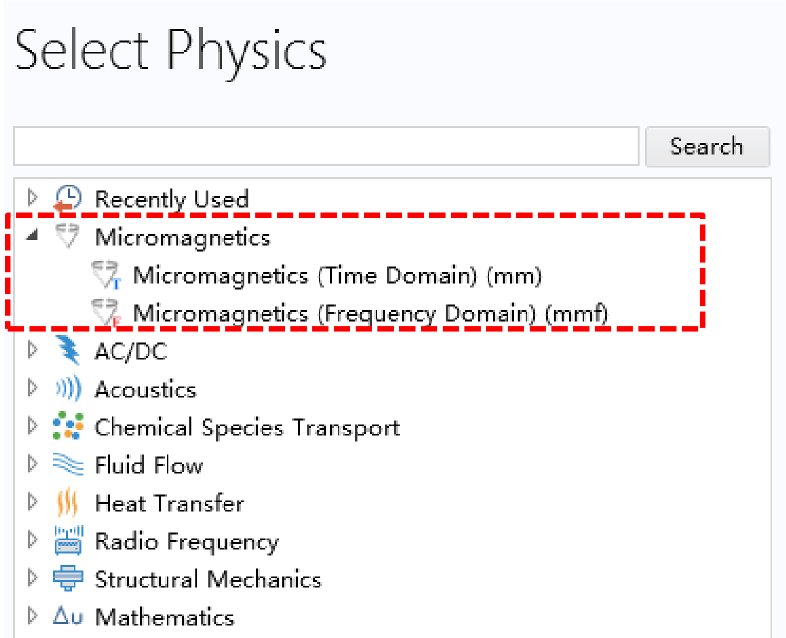
https://cn.comsol.com/blogs/micromagnetic-simulation-with-comsol-multiphysics/



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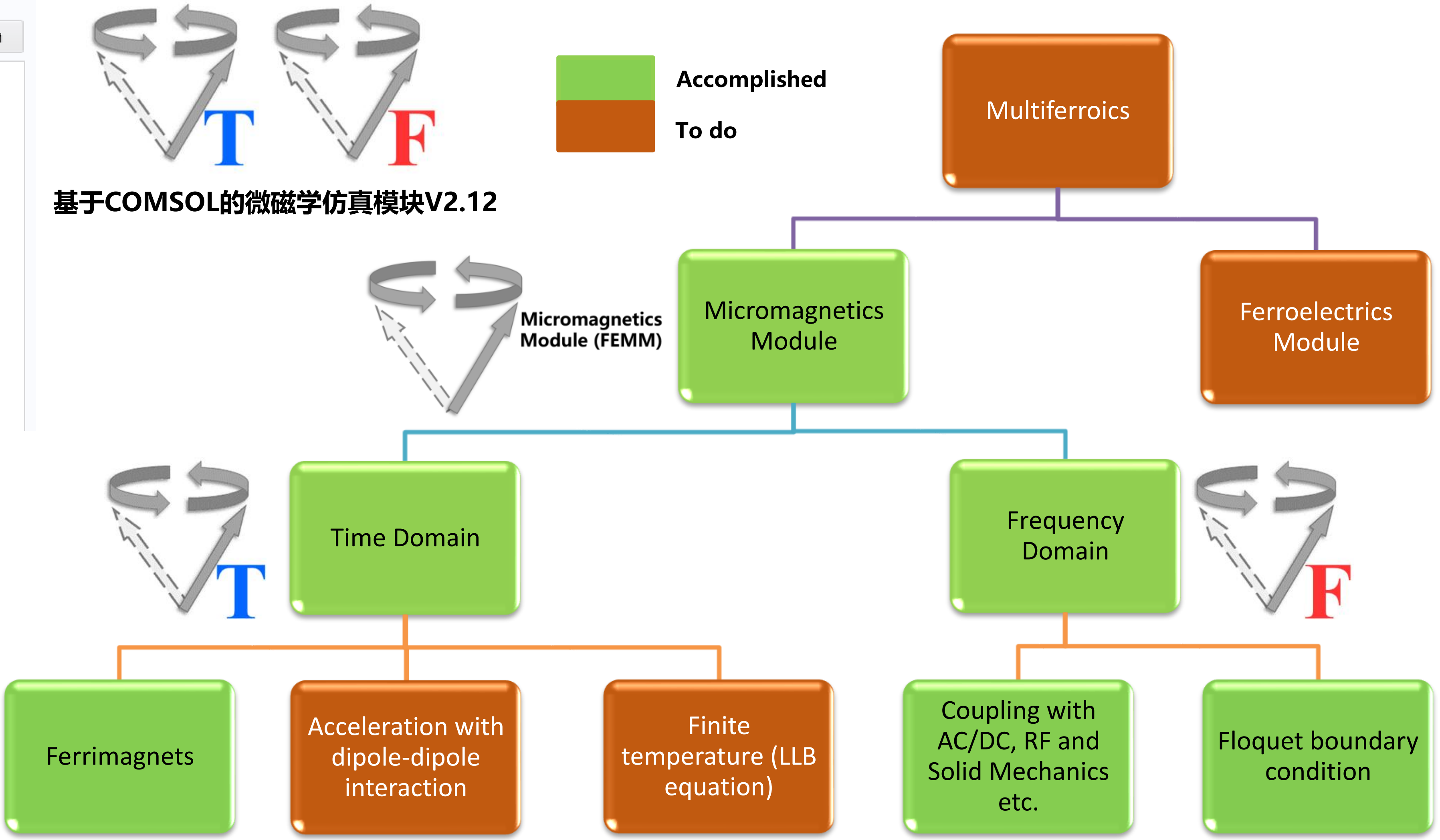

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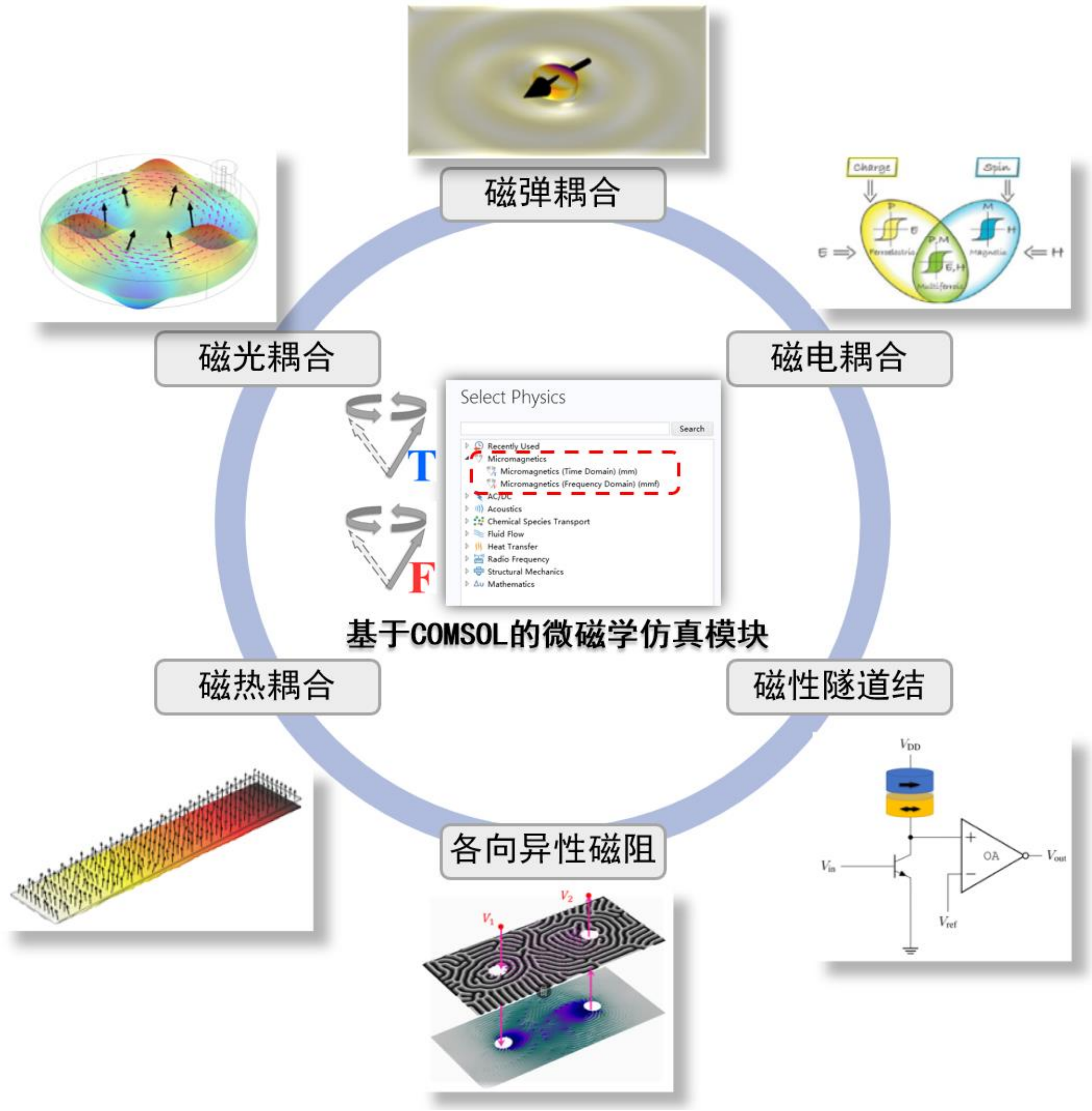

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