Recent Developments in FORC-based Magnetic Modeling

1. **Spin Wave Renormalization of Finite Element Modeling of Magnetic Reversal for FORC applications**

2. **Time dependent FORC analysis**

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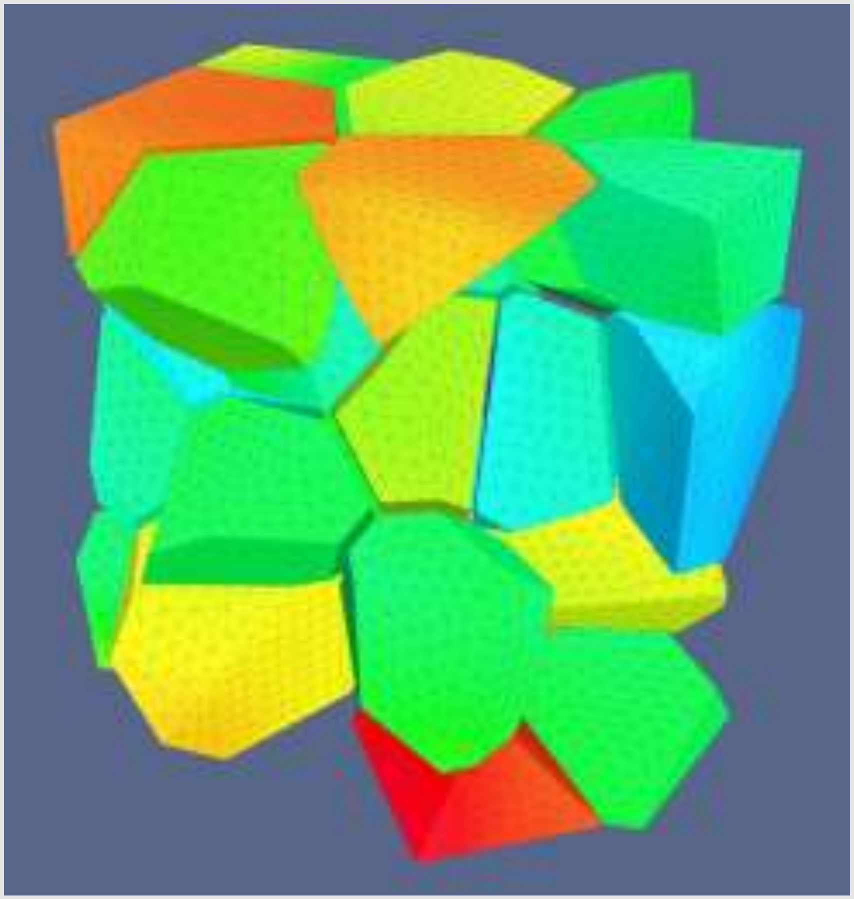
Finite Element Micromagnetism: Fluctuations modify parameters



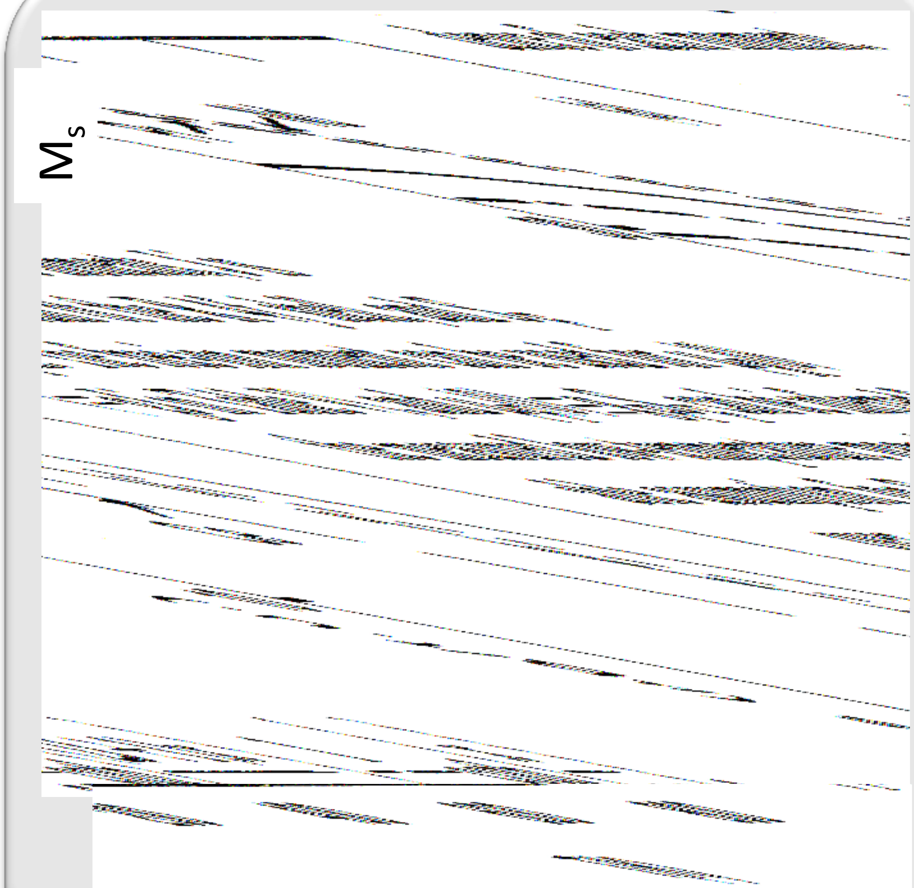
$Nd_2Fe_{14}B$: Schrefl 2015

Finite element simulations are the standard for high quality micromagnetic modeling. Such modeling is the basis for many FORC simulations as well.

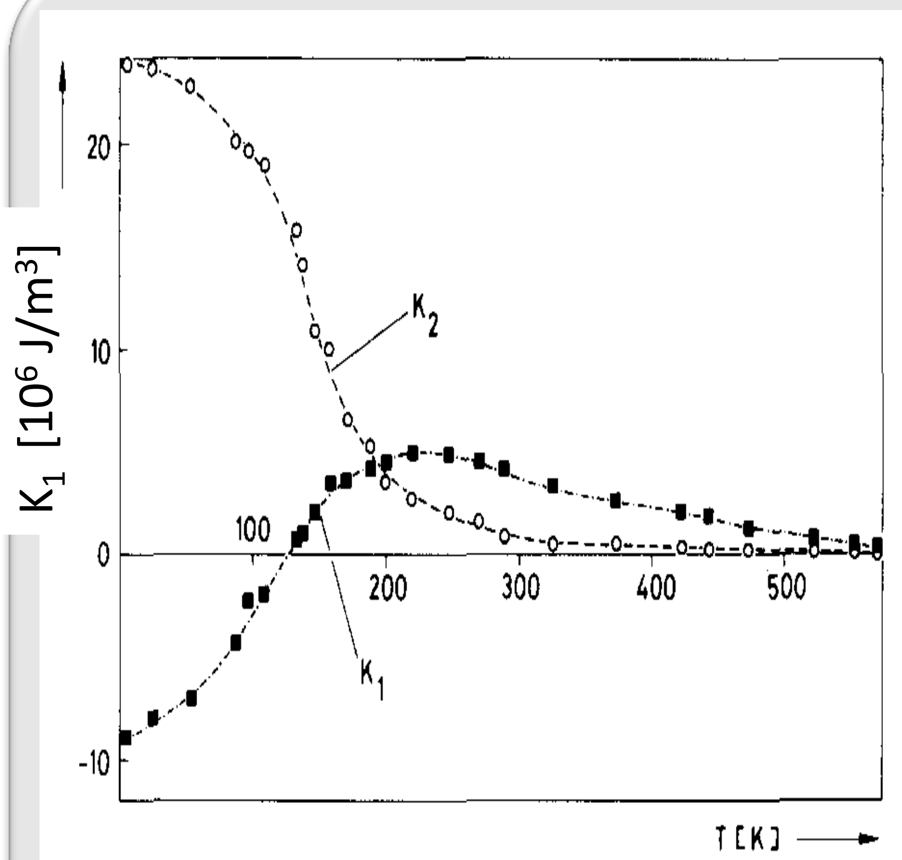
<u>But: what parameters to use</u>?
* Microscopic, from ab initio?
* Experimental, from measurements?
* Thermally reduced?

These differ from each other by the different classes of fluctuations they include

Fluctuations reduce $M_s(T)$ and $K(T)$ from their T=0 values

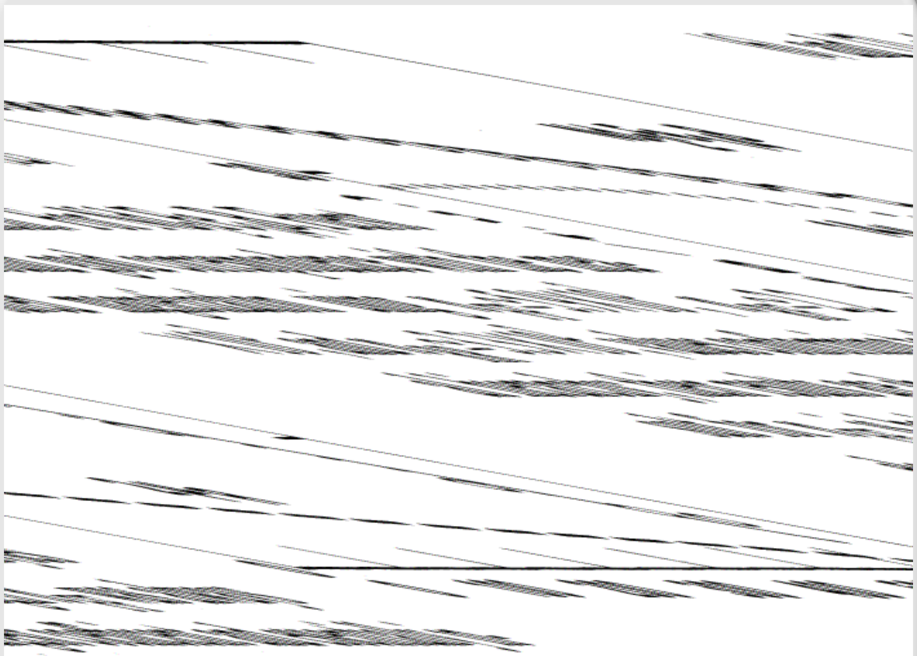


Herbst, 1991

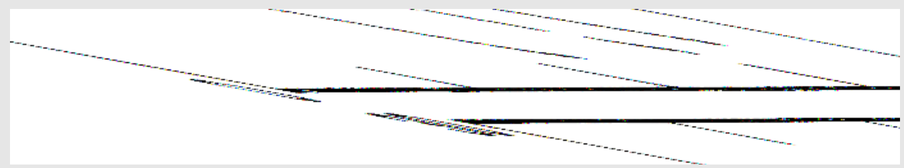


Durst, 1986

Fluctuation Classes: Spatially independent spins

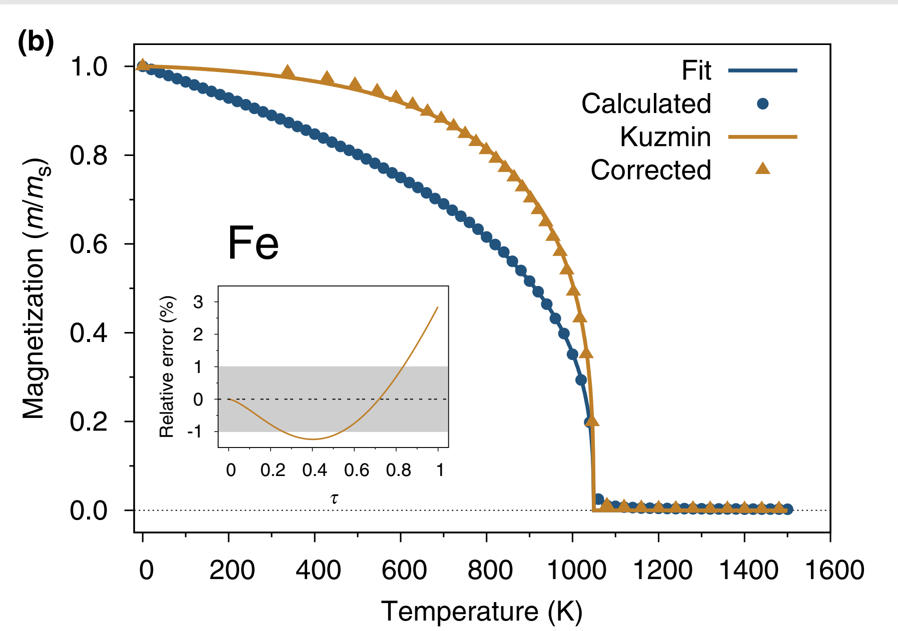


Low T: RE and Fe spins in two sublattices, coupled through molecular field only. Spins assumed to fluctuate spatially independently



Fuerst, 1986

Fluctuation Classes: Collective Spin Waves



Evans, Chantrell 2015

Low T: collective spin waves

* classical

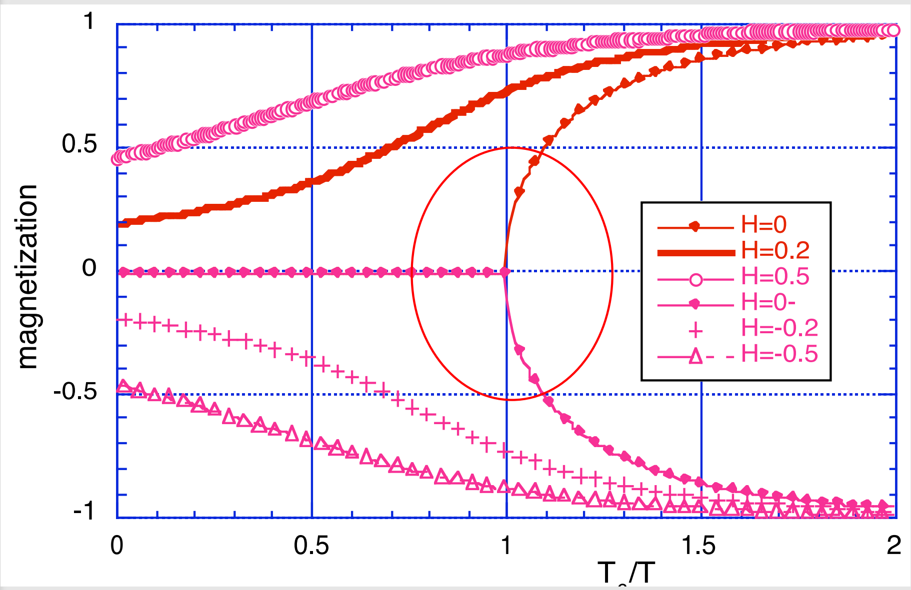
$$m_c(T) = 1 - \frac{k_B T}{J_0}\frac{1}{\mathcal{N}}\sum_{\boldsymbol{k}}\frac{1}{1-\gamma_{\boldsymbol{k}}} \approx 1 - \frac{1}{3}\frac{T}{T_c}$$

* quantum:

$$m_q(T) = 1 - \frac{1}{3}s\left(\frac{T}{T_c}\right)^{3/2}$$

* Kuzmin interpolation from perturbative spin waves to critical behavior

Fluctuation Classes: Collective Critical

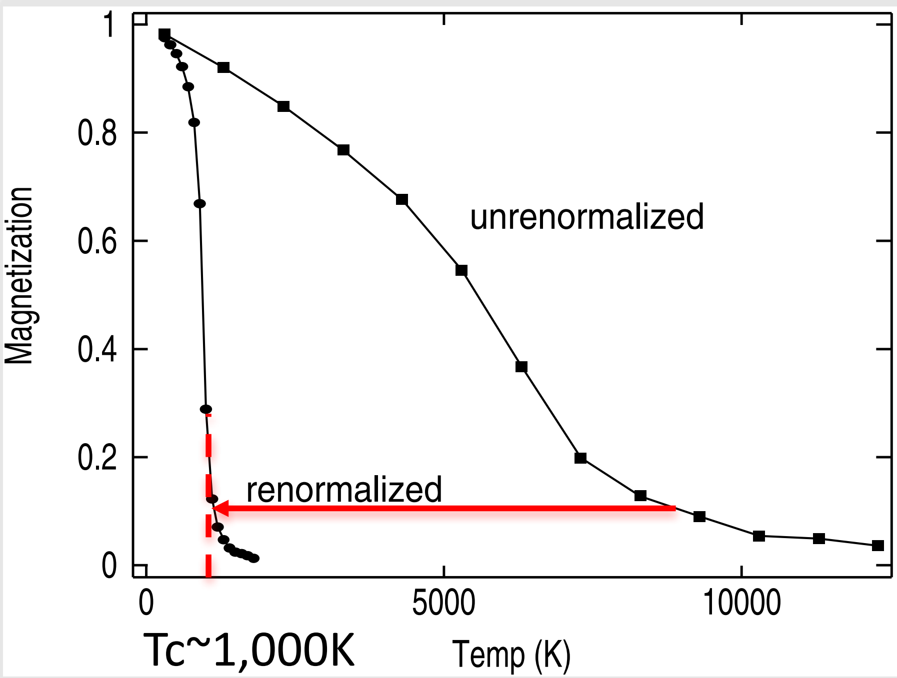


* In critical region close to Tc: Collective critical spin fluctuations.

* Theoretical framework: Renormalization and scaling of the Ginzburg-Landau–Wilson theory.

* Starting from atomic scales, integrate out spin fluctuations to a cutoff length ***L*** and represent the integrated-out fluctuations by an ***l=ln(L)*** dependent renormalization/scaling of the parameters ***g(l):*** $\frac{\partial g}{\partial l} = \beta(g(l))$

Renormalization/Scaling theory of Micromagnetics



Renormalized FEM: Tc becomes realistic

Grinstein, Koch, PRL, 2003

Finite element micromagnetics (FEM) gets Tc very wrong for classes of materials, such as permalloy

Reason: FEM parameters are taken from microscopic values, assuming all spins within finite element cell are fully aligned.

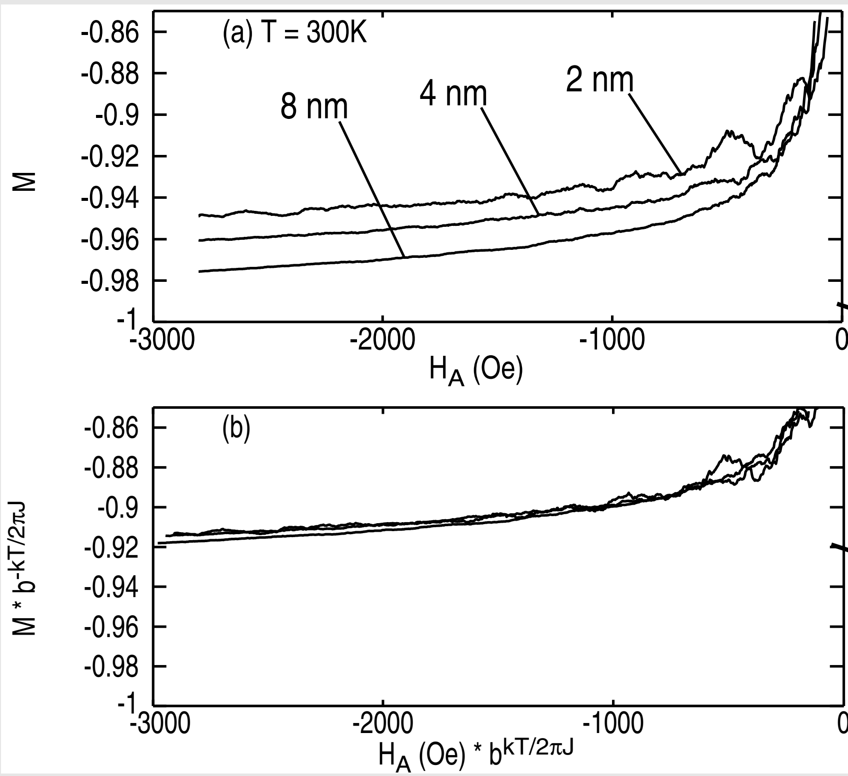
Idea: renormalize the microscopic parameters with spin wave fluctuations of wavelengths smaller than ***L***: "integrate out spin fluctuations to length ***L***"

$$E(\{\vec{S}\}) = \frac{J}{2}\int d^d x (\nabla \hat{s}(\vec{x}))^2$$

$$\partial T/\partial l = -\epsilon T + aT^2$$

all spins aligned **SW fluctuations**

Renormalization/Scaling theory of Micromagnetics



Grinstein, Koch, PRL, 2003

Renormalization in magnetic field ***h***

$$dT(l)/dl = [-\epsilon + \boldsymbol{I}(T(l), h(l))]T(l),$$
$$dh(l)/dl = 2h(l),$$

FEM simulation of magnetization with cell sizes ***L***=2, 4, and 8nm gives **cell-size dependent results.**

FEM with same ***L***=2, 4, and 8nm cell sizes but performed with renormalized parameters gives **cell-size independent results.**

Renormalization/Scaling theory of Micromagnetics

Renormalization with anisotropy g

$$
\begin{aligned}
dT(l)/dl &= [-\epsilon + K(T(l), h(l), g(l))]T(l),\\
dh(l)/dl &= 2h(l),\\
dg(l)/dl &= [2 - 2K(T(l), h(l), g(l))]g(l),
\end{aligned}
$$

Grinstein, Koch, PRL, 2003

Limitations:

(-) FORC: Reversal is different from criticality

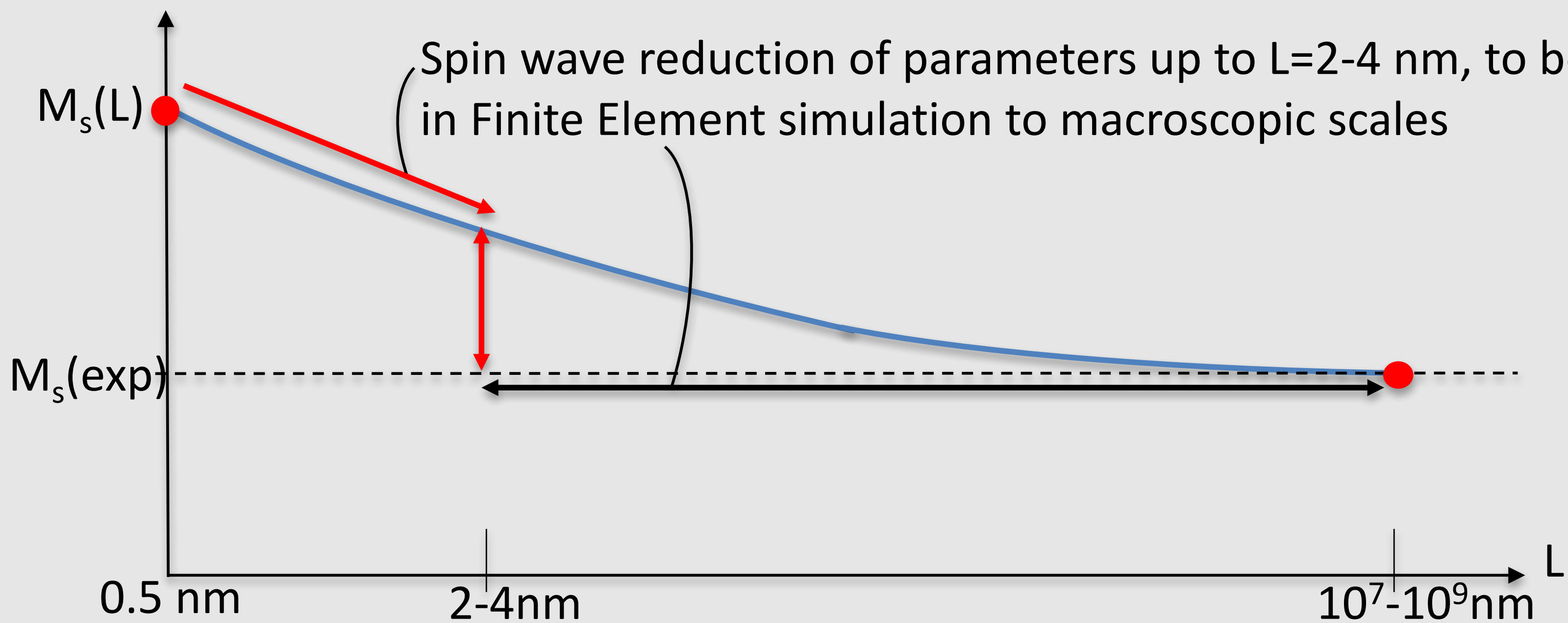
(-) Classical spins

(-) Renormalization approximation: keep only leading logarithms

(-) Geometry approximated as isotropic

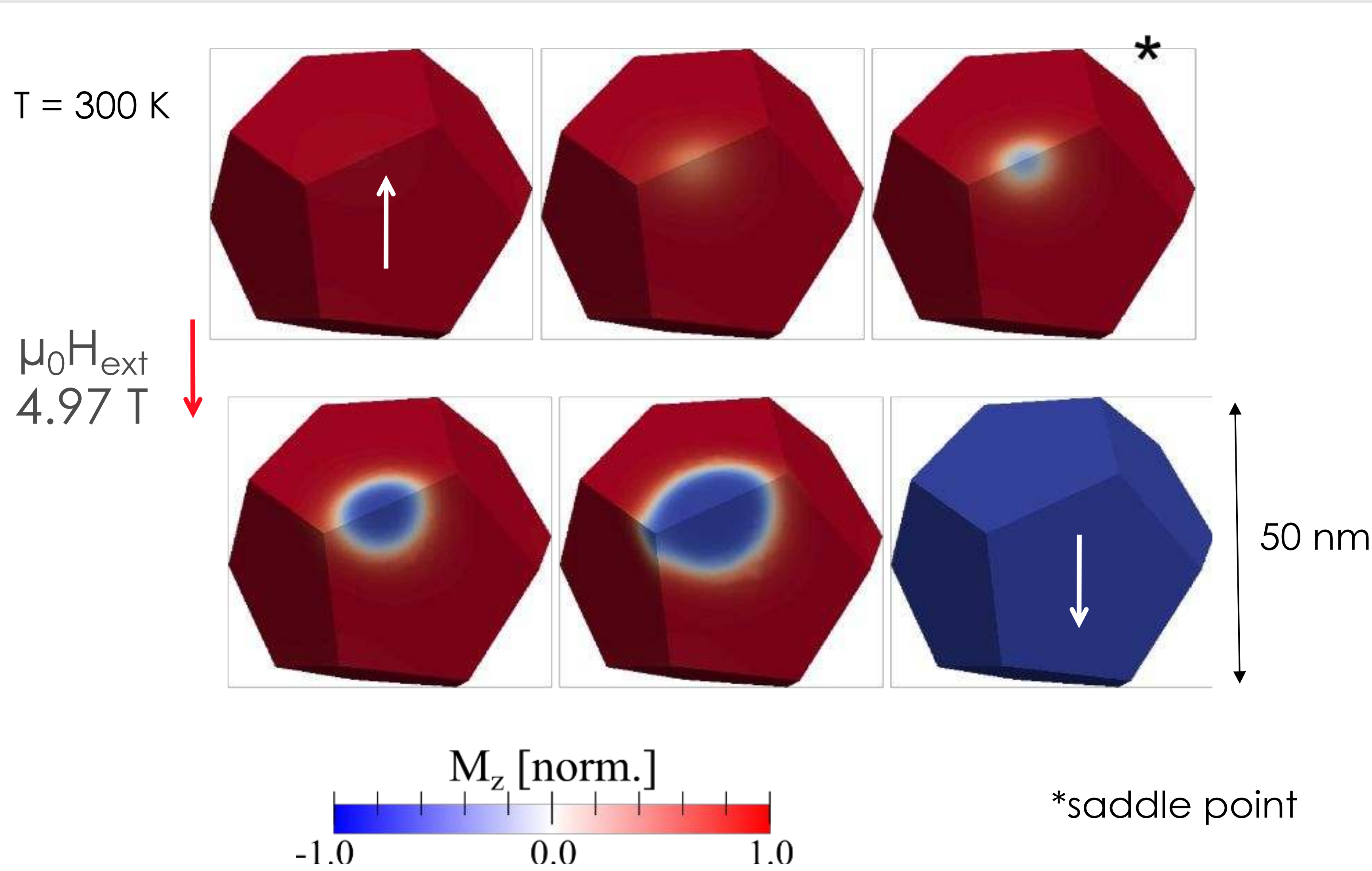
(-) Accurate in 2+ε dimension, becomes less reliable in d=3.

Grinstein: Renormalization by Spin Wave Fluctuations from microscopic to FE scales

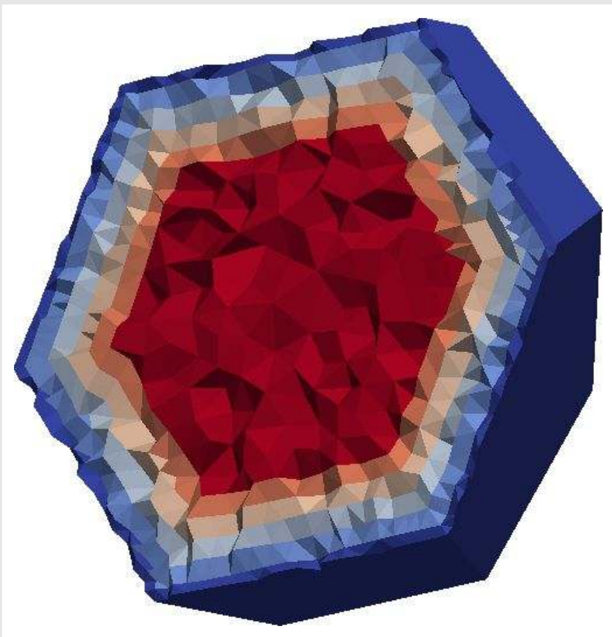


1. Atoms in unit cell	2. Spin waves in FE cells	3. Micromagnetic simulation	4. Macroscopic
Ab initio	***Analytic/RG***	***Finite Element***	***Experiments***

Adaptation for FORC: Reversal is governed by domain wall-mediated nucleation, not spin waves



Reversal simulation by Finite Element Micromagnetics. But what parameters to use?



Activation volume:

$$v = -\frac{1}{\mu_0 M_s} \frac{dE}{dH}$$

For $Nd_2Fe_{14}B$: V=148 nm^3, linear size L~5nm.
L set by domain wall thickness d_{DW}

To capture Domain Wall-mediated reversal, FE cells of size ~2 nm are used at boundaries.

Results are sensitive to FE cell size.

Idea from Renormalization group:

(1) Integrate out Spin Wave fluctuations from atomistic scales to FE cell sizes

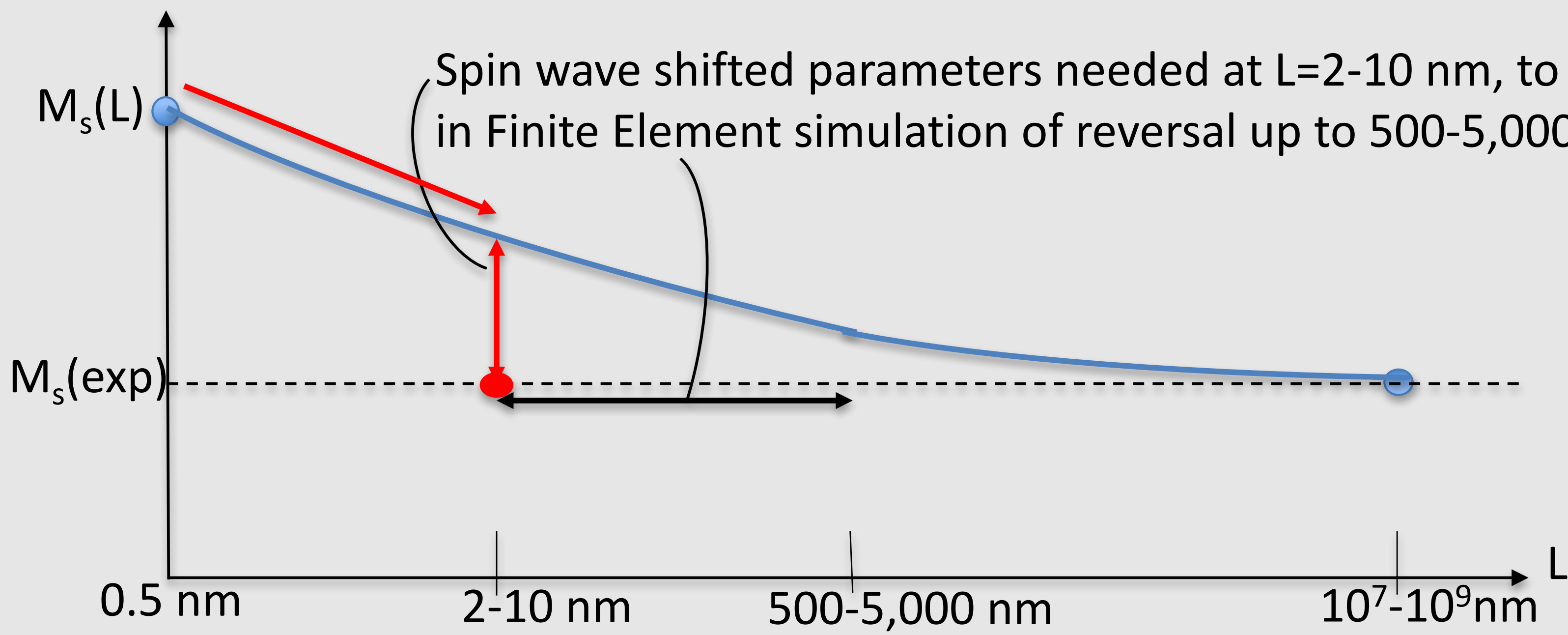
(2) Represent the SW fluctuations through cell-size dependent FE parameters

Advantages:

(1) Capture previously ignored physics

(2) Reduce/eliminate cell size dependence of results

Hierarchical scales of Micromagnetic simulations of magnetic reversal

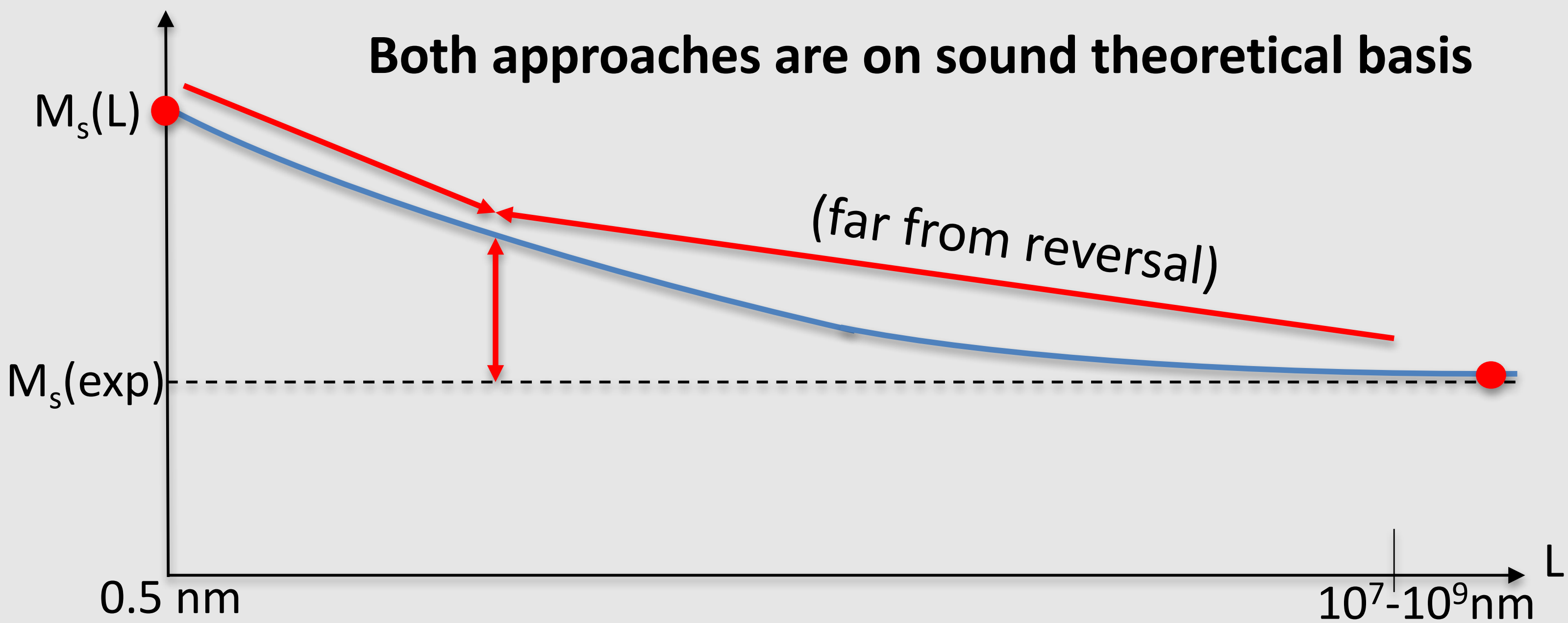


1. Atoms in unit cell	2. Spin waves in FE cells	3. Nucleation, reversal by domain walls	4. Average interactions, $H_K=\alpha K-N_{eff}M$	5. Macroscopic
Ab initio	***Analytic/RG***	***Finite Element***	***Mean field***	***Experiments***

$Nd_2Fe_{14}B$ Microscopic scales: ab initio results cover a wide range

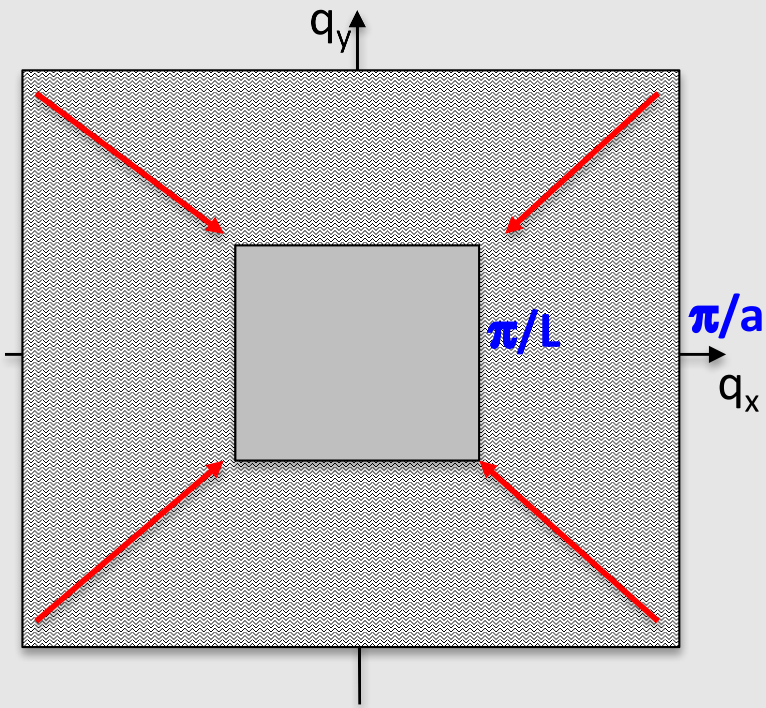
Herbst 1991

Spin Wave Fluctuation Corrections: Relative to Microscopic or Macroscopic Scales?

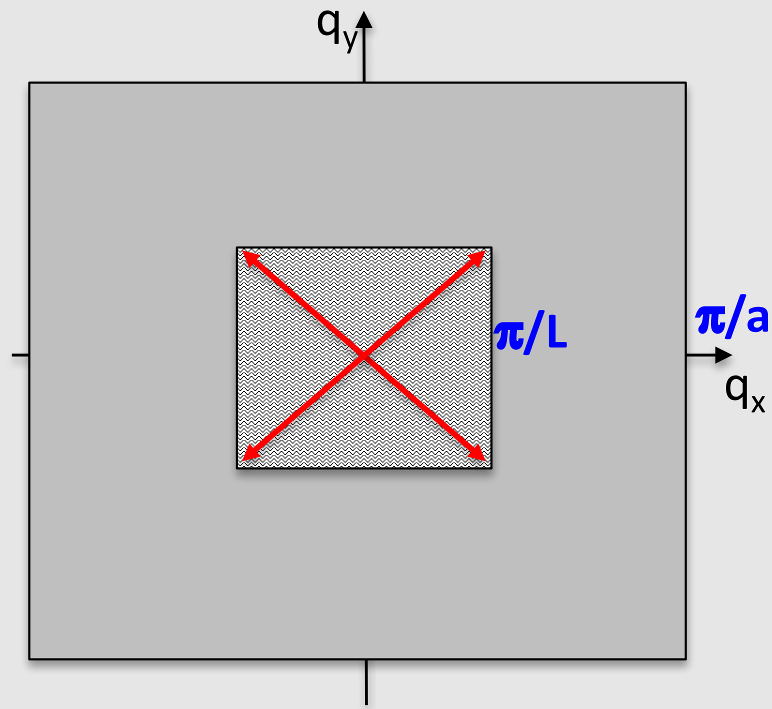


1. Atoms in unit cell	2. Spin waves	3. Macroscopic
Ab initio	***Analytic/RG***	***Experiments***

Spin Wave Fluctuation Corrections to Microscopic and to Macroscopic scales

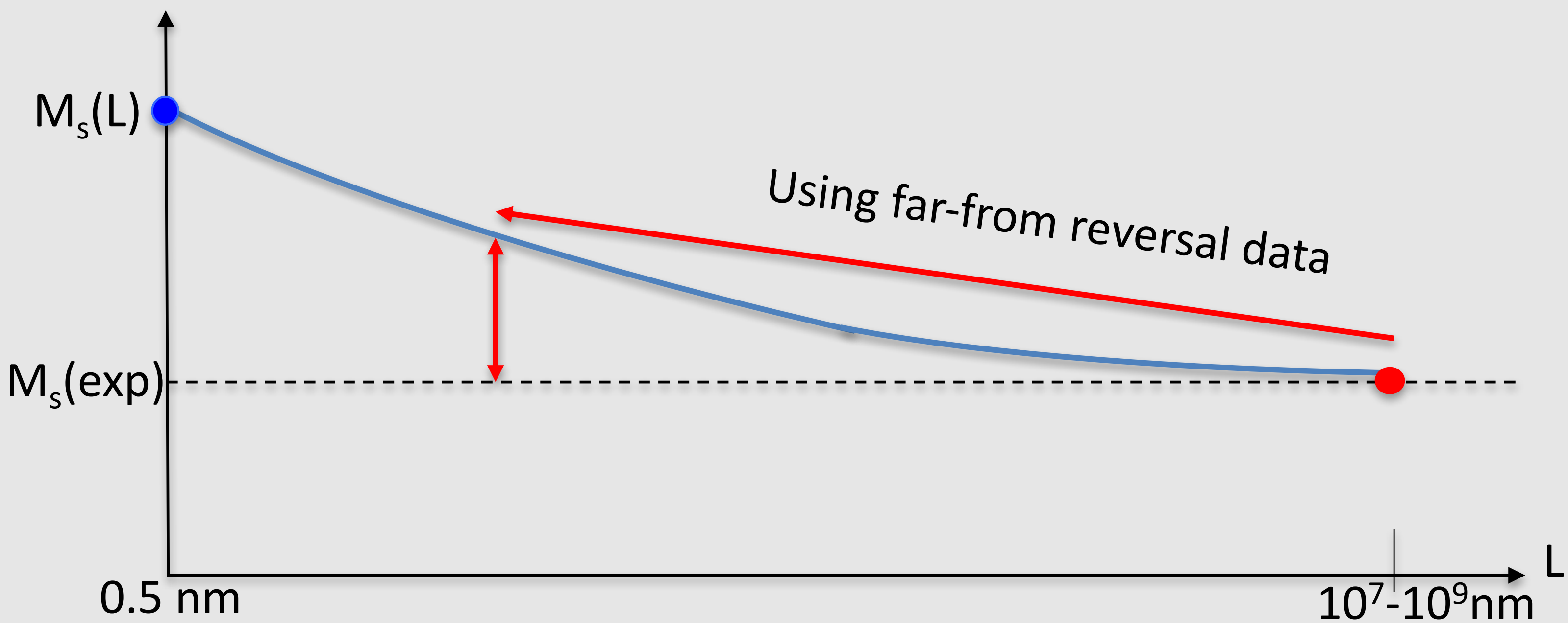


From **microscopic** to FE cell size L



From **macroscopic** to FE cell size L

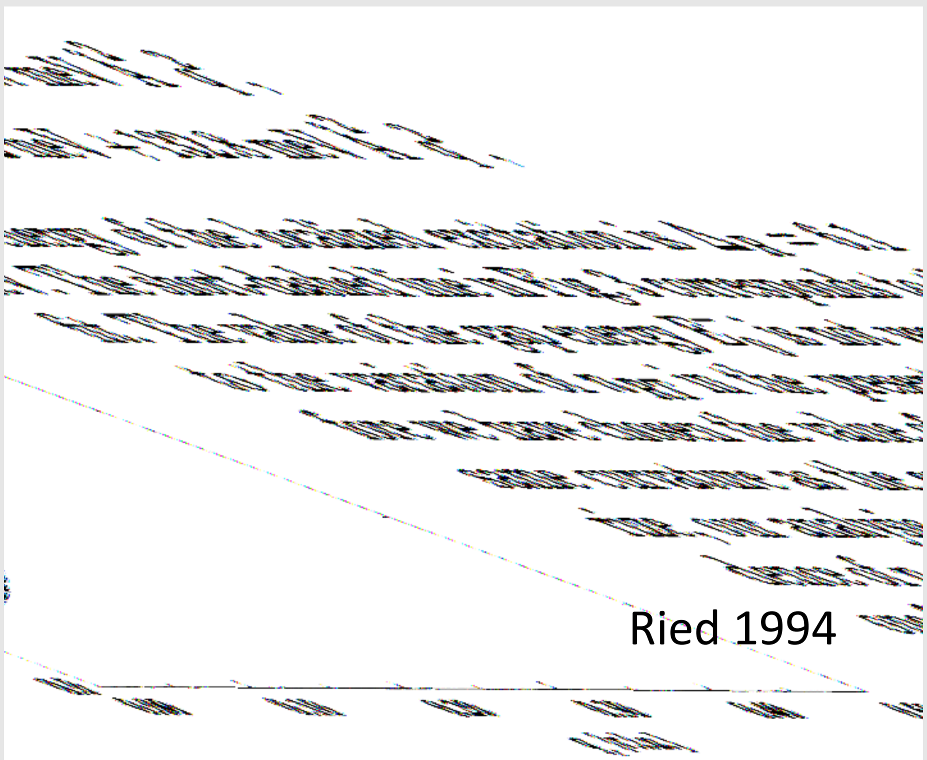
Anchor Spin Wave Fluctuations at Macroscopic Scales



1. Atoms in unit cell	2. Spin waves	3. Macroscopic
Ab initio	***Analytic/RG***	***Experiments***

Spin-Wave Renormalization of Finite Element Cell Parameters: $Nd_2Fe_{14}B$

$$\frac{M(L)}{M(exp)} = 1 + \frac{2\mu_B}{M(exp)}\frac{V}{(2\pi)^3}\iiint_{-\frac{\pi}{L}}^{\frac{\pi}{L}} dk \left[exp\left(\frac{E(k)}{kT}\right) - 1\right]^{-1}$$

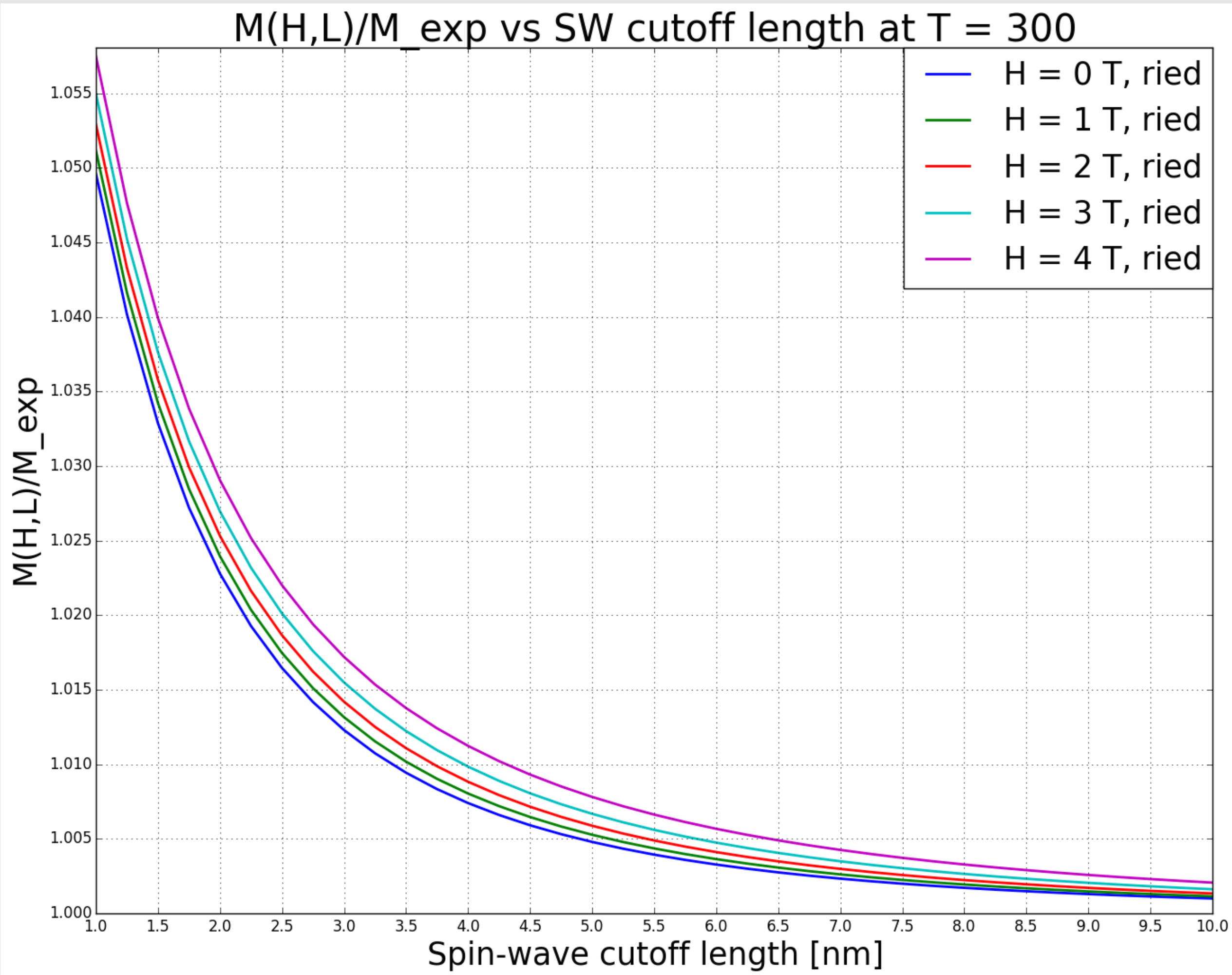


Ried 1994

T(K)	300K	450K
μ_0Ms(T)	1.61	1.29
A(pJ/m)	7.7	4.9
K (MJ/m^3)	4.3	2.9

Far from coercive field: Durst 1986

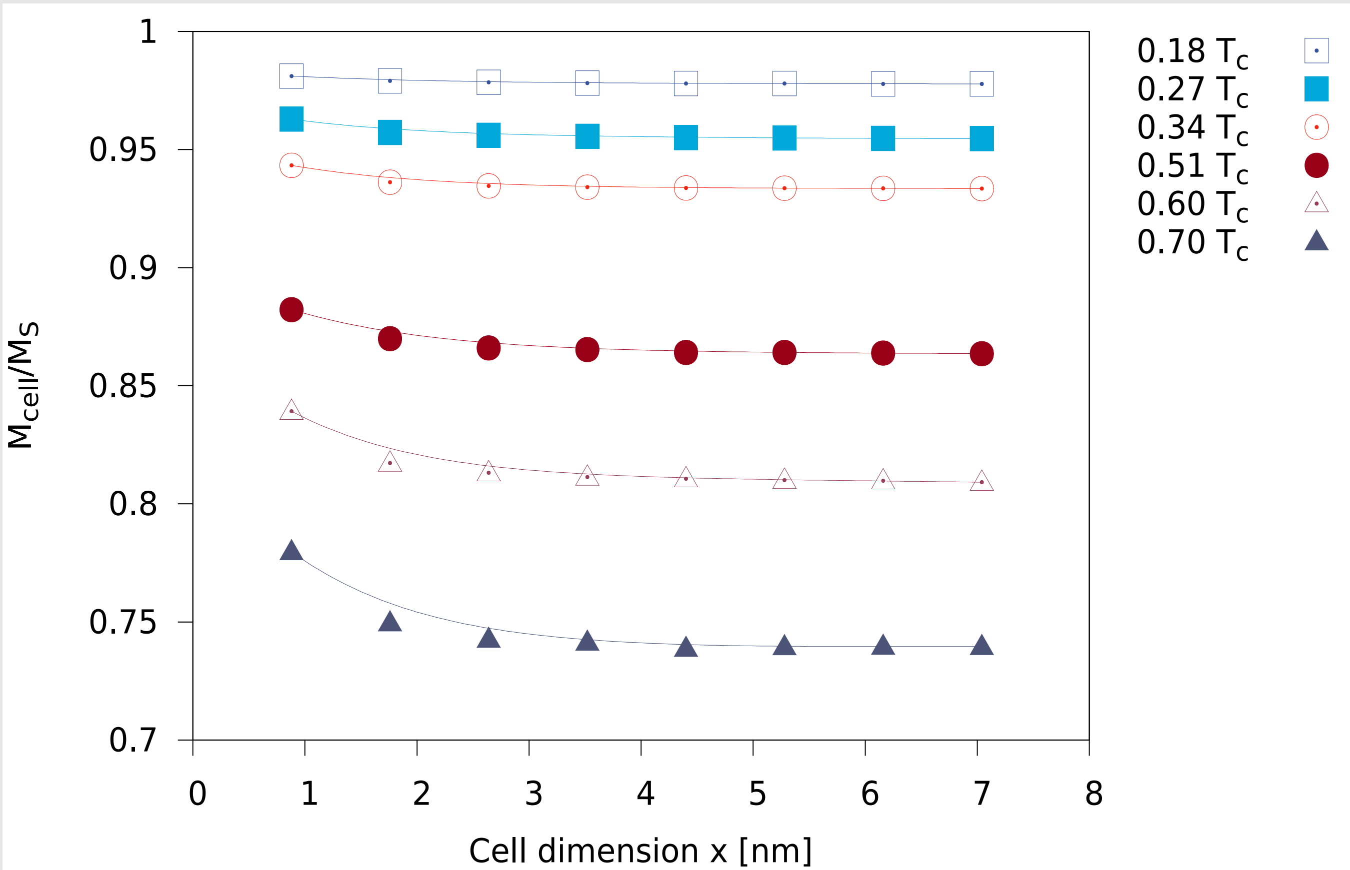
$Nd_2Fe_{14}B$: Magnetization M(H,L) at T=300K



Represent magnetic field with Zeeman gap.

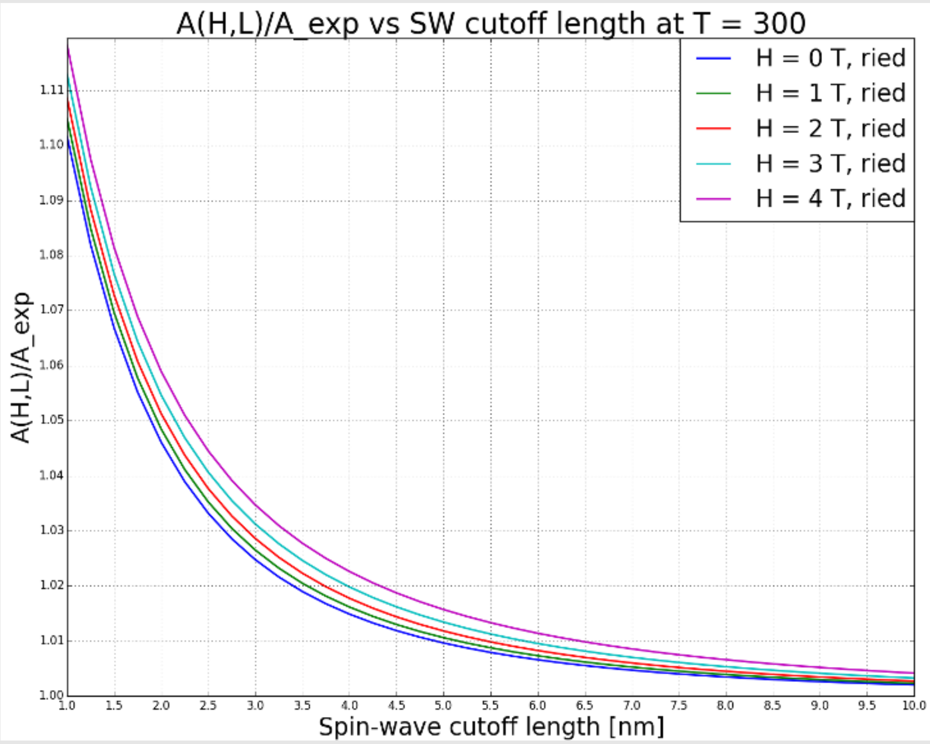
FE simulation has to use 5.5% higher M(L) values than M(exp) when simulating L=1nm cells

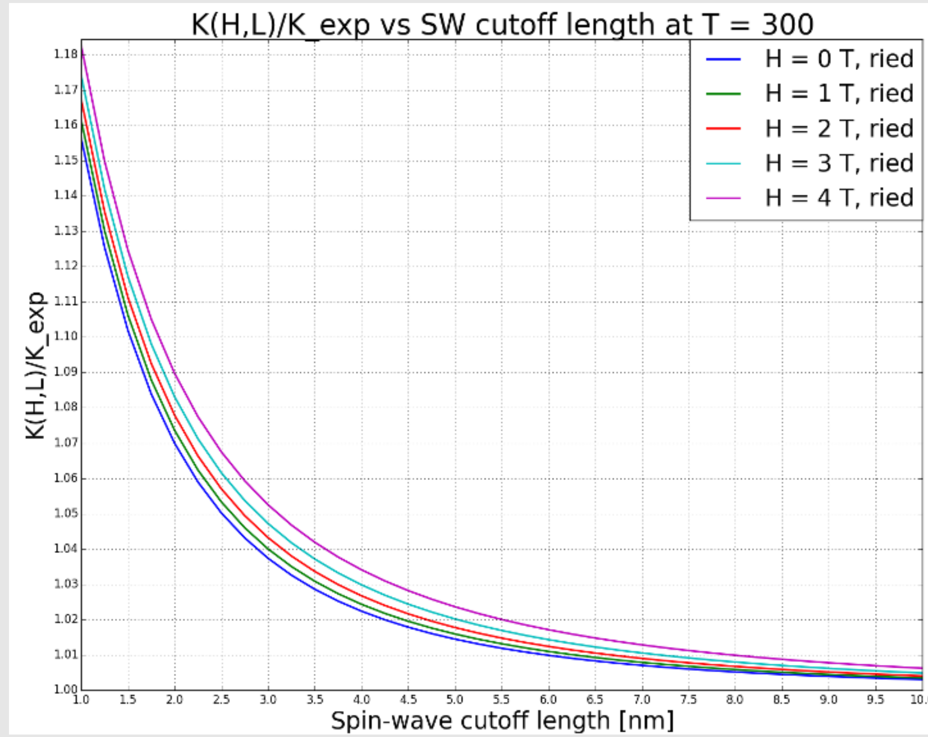
Spin Wave Fluctuations by classical spins



Chantrell simulated classical spin systems. Also reported 5-7% size dependent correction of M(L) for cell sizes of L=1nm

$Nd_2Fe_{14}B$: Exchange A(H,L), Anisotropy K(H,L) at T=300K

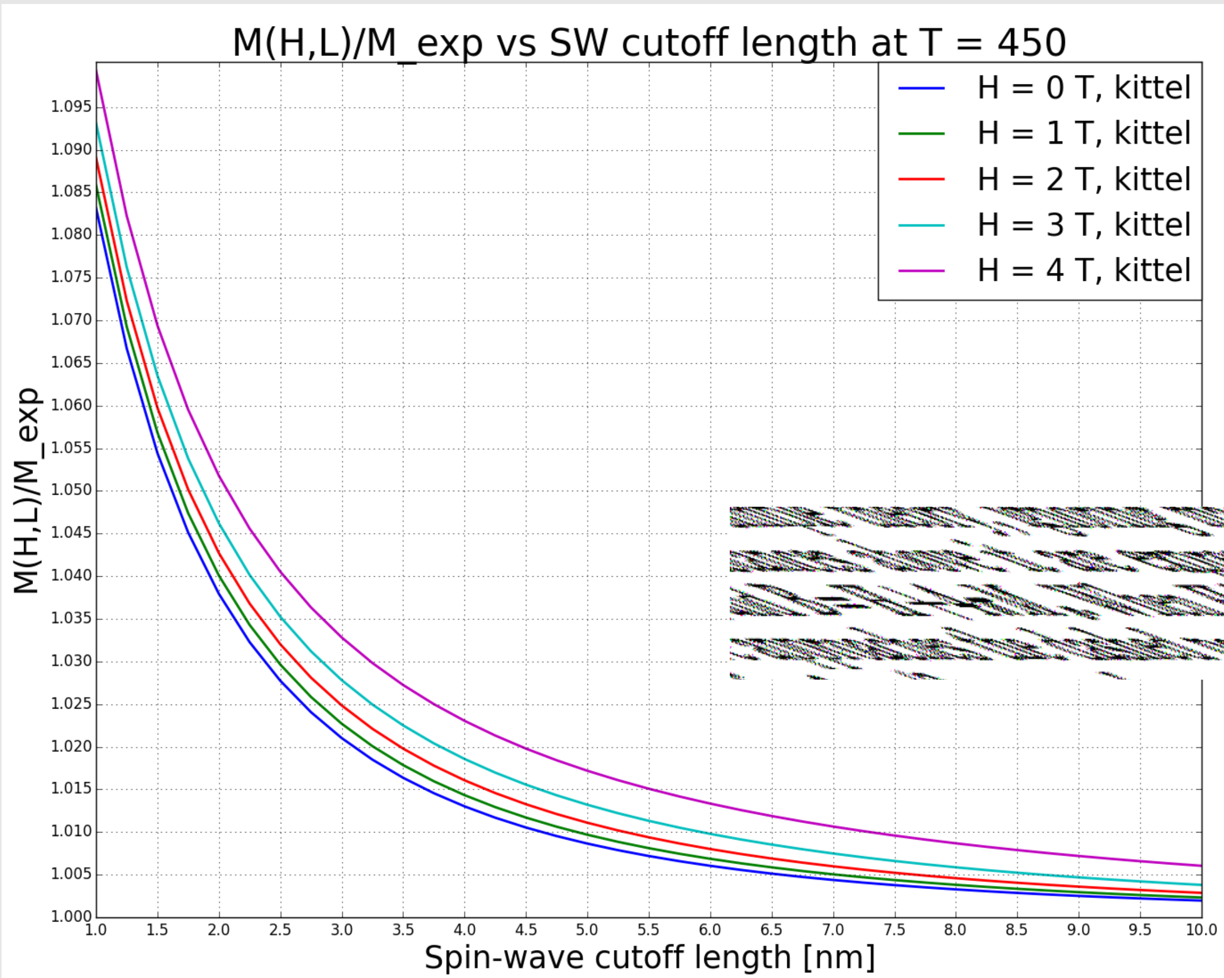




$A \sim M^2$
10% enhancement at L=1nm

$K \sim M^3$ Callen-Callen law
15% enhancement at L=1nm

$Nd_2Fe_{14}B$: Magnetization M(H,L) at T=450K



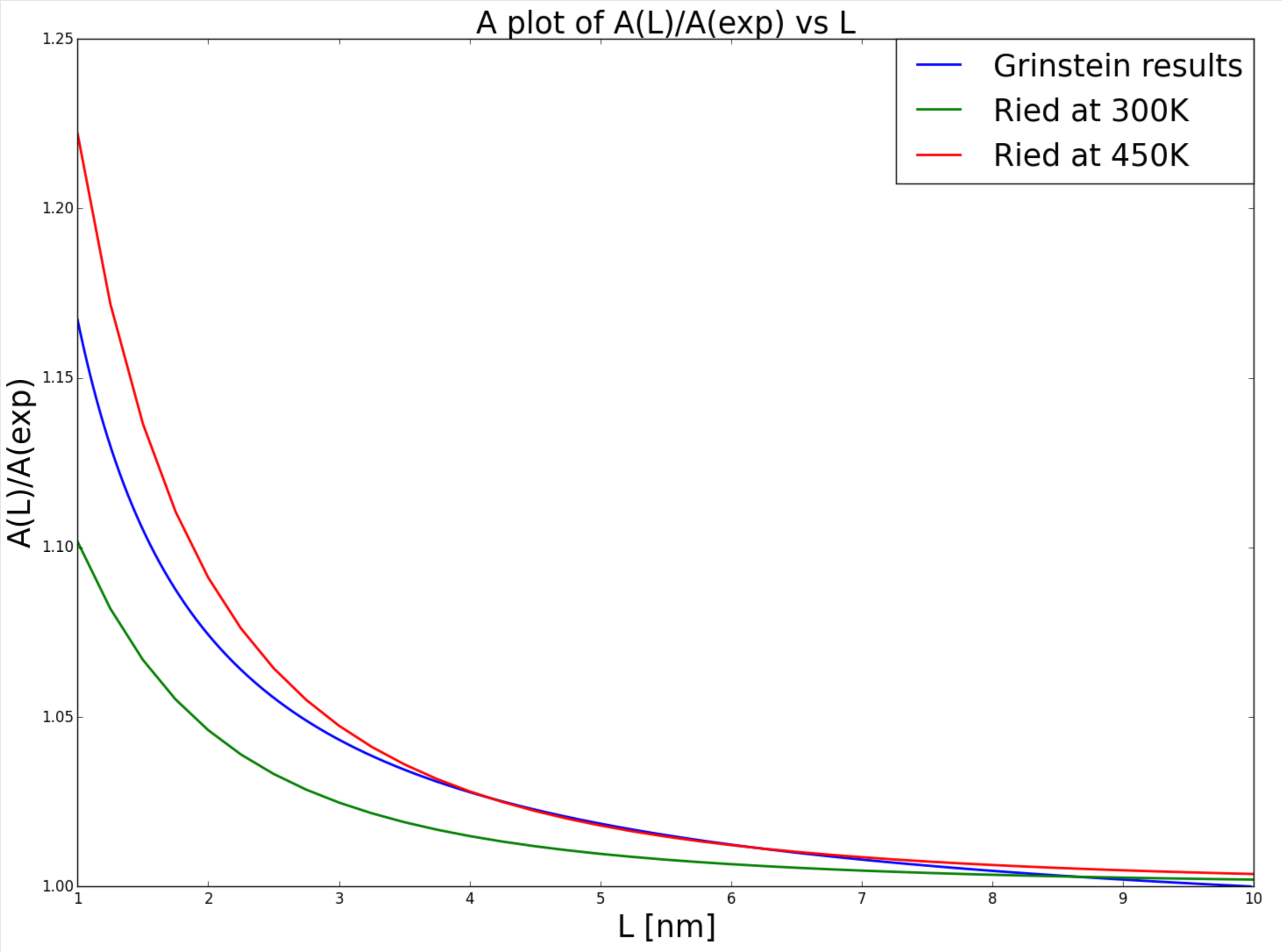
Spin wave spectrum not known at T=450K

We use Holstein-Primakoff-Kittel:

$E(k)=(A_k^2-B_k^2)^{1/2}$

9% enhancement at L=1nm

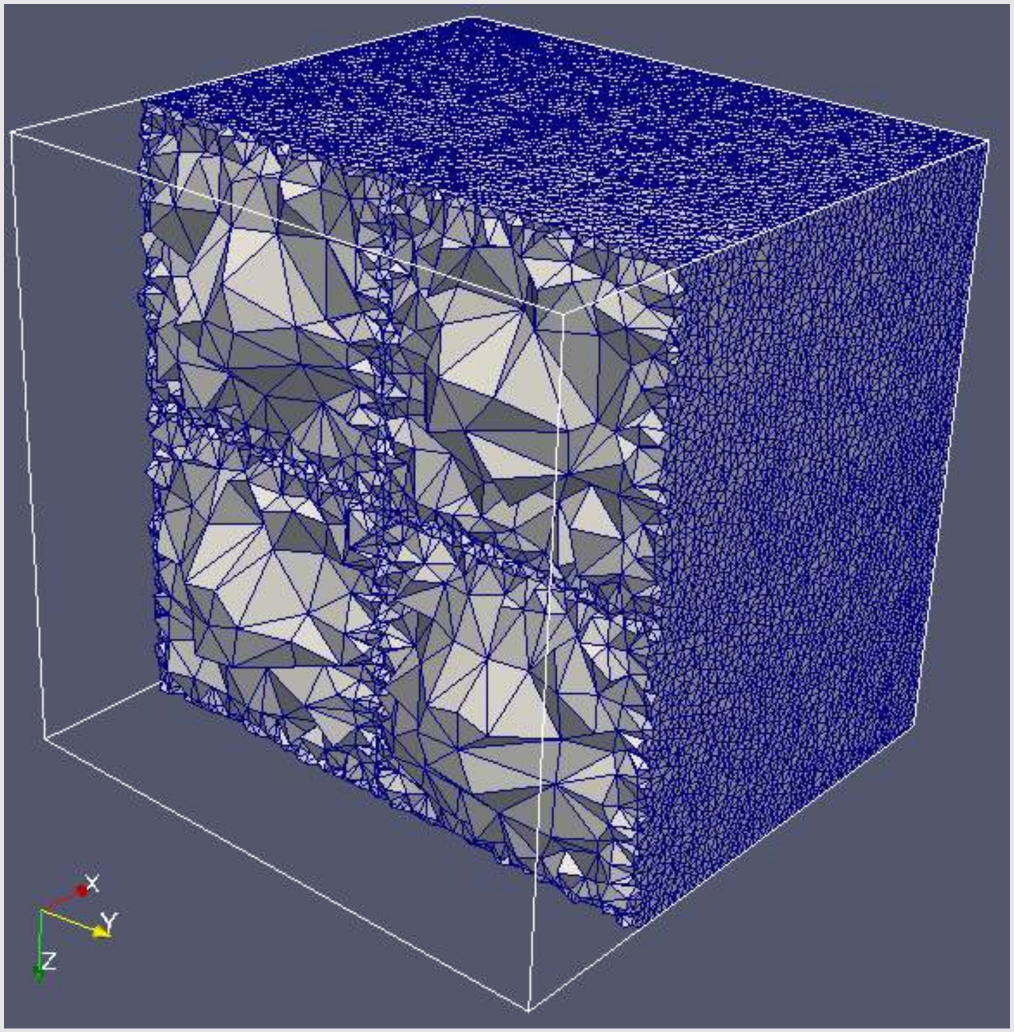
Comparison of Grinstein Scaling theory and Spin Wave Renormalization



Two results show very analogous trends and magnitude

Differences between theories explain differences between results

The Spin-Wave Renormalized Finite Element Simulation of $Nd_2Fe_{14}B$ at T=450K



$Nd_2Fe_{14}B$

$80nm^3$ nanostructured sample,

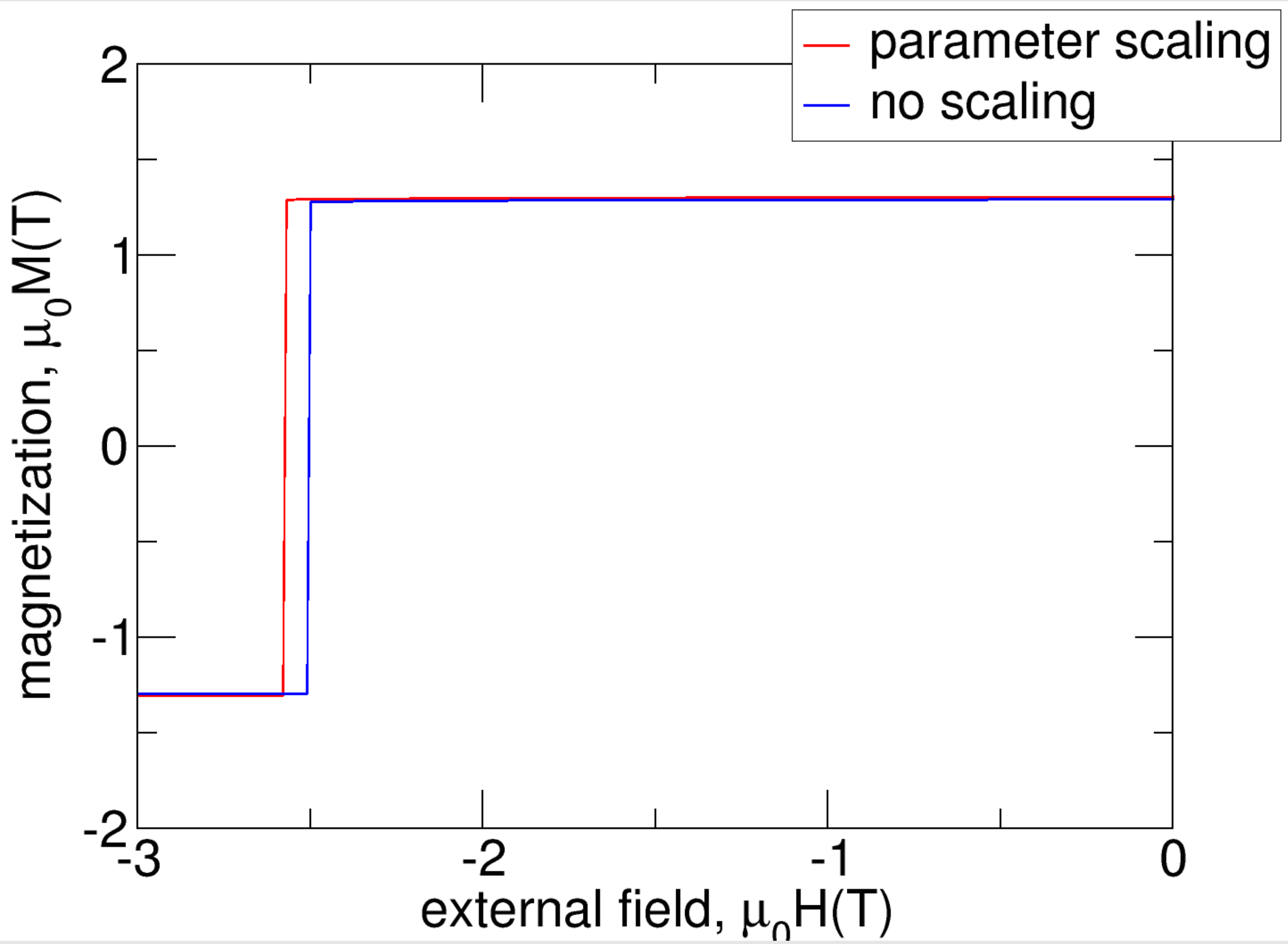
2x2x2 NdFeB blocks

Weak ferromagnetic d=2nm layer between blocks

Cell size at boundary: L=1nm

T(K)	450K
$\mu_0Ms(T)$	1.44
A(pJ/m)	5.7
$K(MJ/m^3)$	2.73

The Spin-Wave Renormalized Finite Element Simulation of $Nd_2Fe_{14}B$ at T=450K



Including Spin Wave Renormalization of the FE parameters increases $\mu_0 H_c$ by 5%, from 2.5T to 2.6T.

2. Time Dependent FORC Analysis

IEEE TRANSACTIONS ON MAGNETICS, VOL. 34, NO. 4, JULY 1998

A Preisach Model for Aftereffect

Edward Della Torre and Lawrence H. Bennett

* Time dependent dynamics of magnetization is governed by the barriers against reversal

* FORC represents barriers very well

* Simple model calculation explains famous logarithmic
  "Sharrock's law" decay

* **Can be used to connect FORC diagrams, measured at t~10^2 sec**
  to time scales of interest:
  10^{-9} sec for recording, and 10^{+9} sec for geological applications

2. Time Dependent FORC Model Calculation

$$m_i(t) = m_i(0) + \Delta m_i \left(1 - \int_0^\infty p_\tau(\tau) \exp(-t/\tau)\, d\tau \right)$$

Magnetization relaxes over barriers that translate to a relaxation time distribution

$$\tau = \tau_0 \exp[(u-h)/h_f], \text{ for } u>v$$

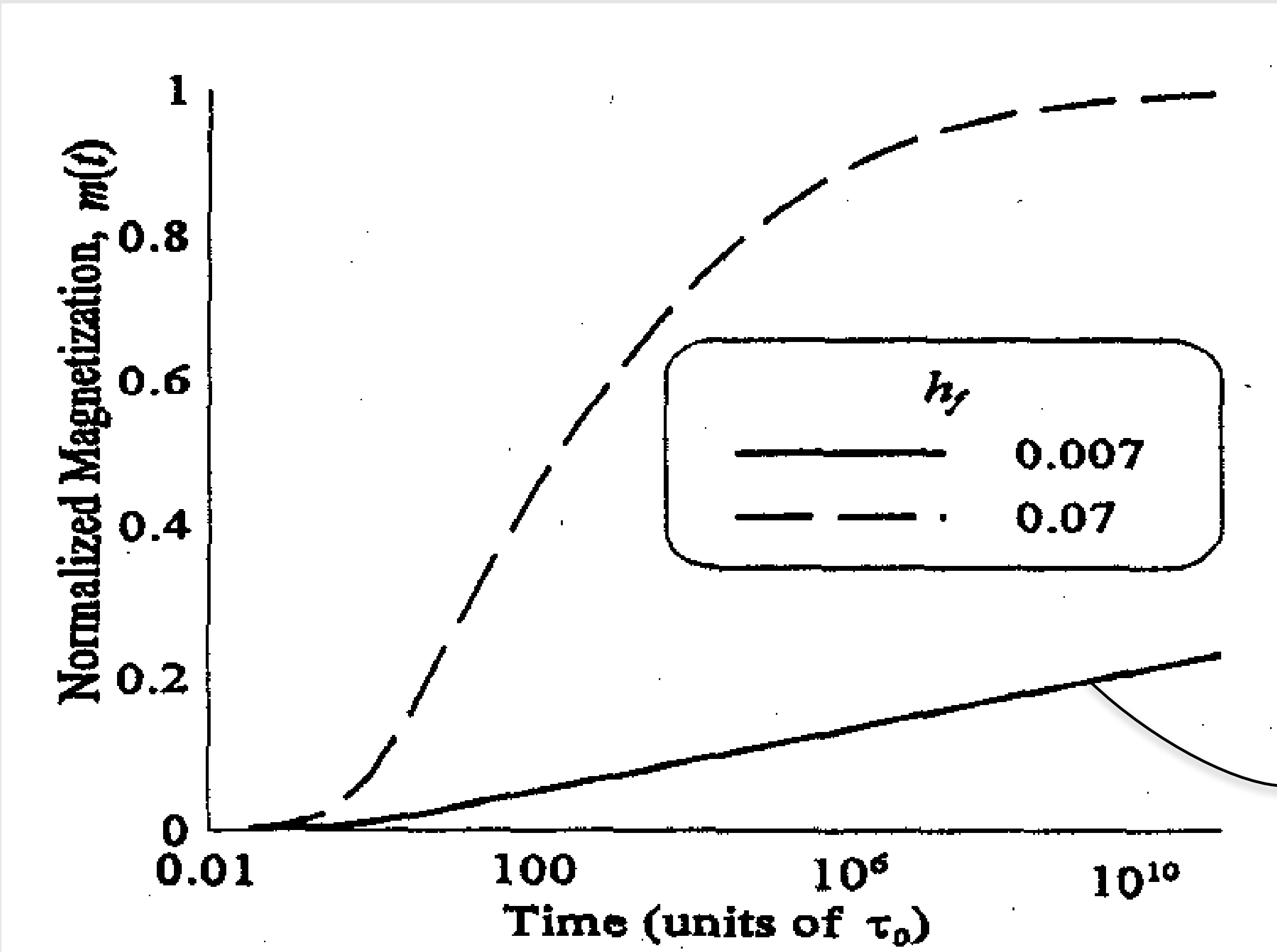
Activated dynamics, with "fluctuation field" ~ *kT*

$$h_f = kT/\mu_0 MV$$

$$p(u) = \exp\left[-(u-\bar{h}_k)^2/2\sigma^2\right] / \sigma\sqrt{2\pi}$$

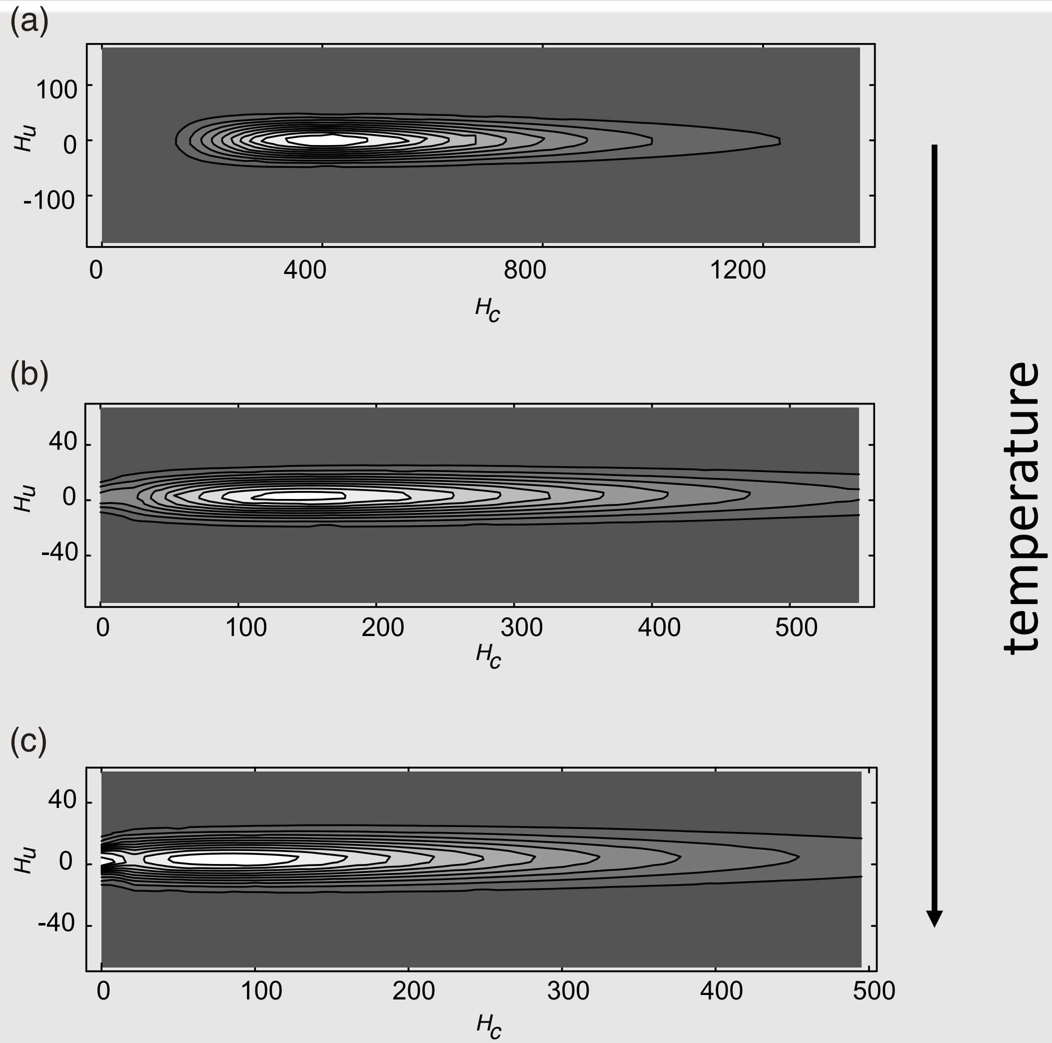
Gaussian FORC distribution of switching fields h_k

2. Recovering Sharrock's $\Delta M(t)$~log(t) law



Sharrock's
$\Delta M(t)$ ~ log(t) law

2. Temperature dependence at fixed time



Pike, Verosub, 2000

Summary

1. Introduced the concept of Spin Wave Renormalized FE cell parameters; developed calculation scheme for these Spin Wave Renormalized parameters
2. Implemented Spin Wave Renormalization-driven cell size dependent parameters into Finite Element modeling
3. Showed that including the Spin Wave Renormalization into Finite Element modeling increases Hc of $Nd_2Fe_{14}N_x$ by ~5% to Hc=2.6T
4. Spin Wave Renormalization much bigger (~ factor 10) for soft materials, e.g. between hard grains, or permalloy