Computational Instrumentation for Material, Nano-, and Condensed Matter Sciences

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Computational Material Sciences Group

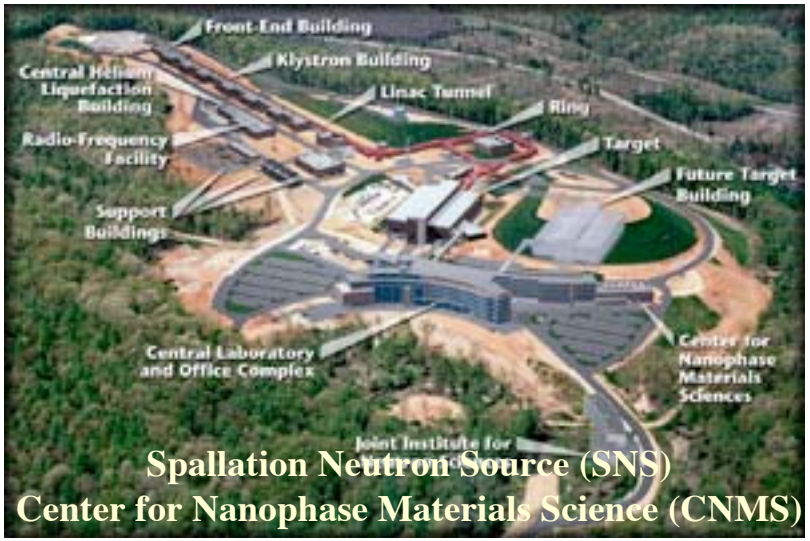
Computer Science and Mathematics Division

New world-class facility will be housing leadership class computers

- **Space and power:**
  - **40,000 ft^2 computer center with 36-in. raised floor, 18 ft. deck-to-deck**
  - **8 MW of power (expandable) @ 5c/kWhr**
- **Classroom and training areas for users**
- **High-ceiling area for visualization lab (Cave, Powerwall, Access Grid, etc.)**
- **Separate lab areas for computer science and network research**

Spalation Neutron Source and Center for Nanophase Materials Sciences

New Approach: facility analogy



User Community

Data Analysis

Facility

Virtual User Center

Materials : Math : Computer Scientists

- *Open Source Repository*
- *Object Oriented Tool Kit*
- *Focused User Laboratories*
- *Education*

User Community

Relevant modeling at ORNL

- **Magnetism, magnetic hetero (nano) structures**
- **Transport: magneto- and molecular electronics**
- **Strongly correlated electron systems**
  - **DFT based electronic structure (LDA, GGA, …, SIC-LSD)**
  - **Spin dynamics / statistics (ab initio, Heisenberg, spin-Fermion)**
  - **Strongly correlated models / effective medium theory (DMFT, DCA)**
- **Structural / mechanical properties:**
  - **Alloy phase stability (nano phases)**
  - **Microstructure evolution**
  - **Radiation effects**
  - **Metallic classes**
  - **Fracture; continuum mechanics (Finite Element Meth.)**
  - **… *and many more* …**
- **Tribology, nano-fluids, polymers**
- **Protein / DNA structure**

Outline

- **Introduction:**
  - **Computational "End-Station" concept for material, nano-, and condensed matter sciences**
- **Selected example "simulations" (theory & computation):**
  - **Modeling assemblies of magnetic nanoparticles**
  - **Spin waves above T_c in Fe**
- **Software development in CCS-MRI and CNMS/NTI**
  - ***Ψ-Mag* toolkit**
  - **XML based I/O**
- **Summary and Conclusions**
  - **Is this useful for data analysis needs at SNS and HFIR?**

Collaborators

- **Computational End-Station:**
  - **Malcolm Stocks (M&C Division) and Peter Cummings (CNMS/NTI)**
  - **Doug Lowndes (CNMS)**
- **Ongoing leadership computing applications**
  - **Thomas Maier and Gonzalo Alvarez (Wigner Fellows)**
  - **Mark Jarrell (U. of Cincinnati) and Elbio Dagotto (UT/ORNL)**
  - **Trey White and Mark Fahey (CCS)**
- **Modeling assemblies of nanoparticles and PsiMag development**
  - **Hwee Kuan Lee and Greg Brown (partly funded by CMSN)**
  - **Experimentalists (Korey Sorge, Jim Thompson, et al.; Jian Shen and his group)**
- **Spin waves in paramagnetic Iron**
  - **Xiuping Tao and Davis Landau (UGA), Malcolm Stocks**
- **XML and Software analysis and quality control**
  - **Mike Summers (ORNL), Tom Swain (UT), and Greg Brown**
- **AND MANY OF THEIR COLLABORATORS**

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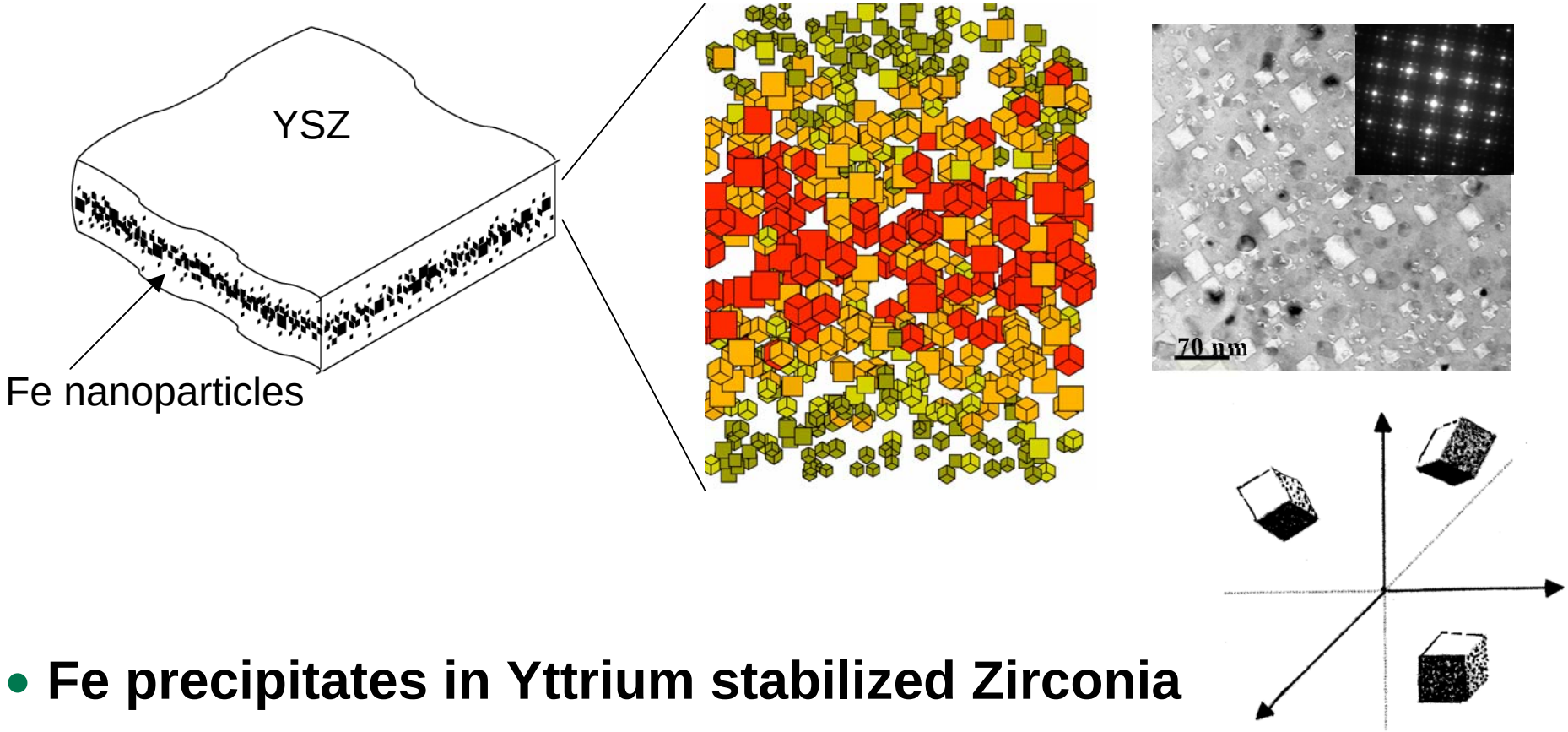
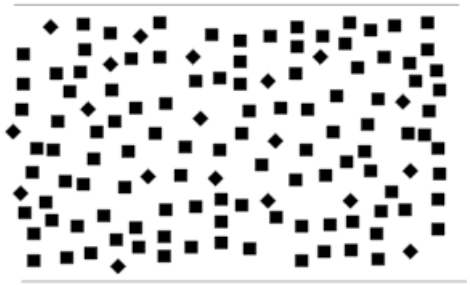
Fe nanoparticle in Y-stabilized Zirconia



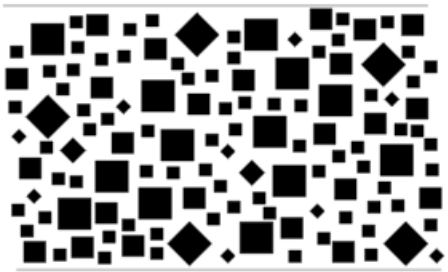
- **Fe precipitates in Yttrium stabilized Zirconia**
- **Particles are coherent with matrix**
- **Packing fraction, orientation, and size distribution known**

Constructing the Model

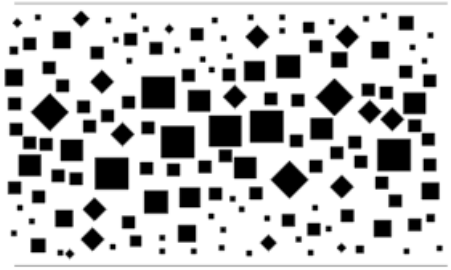
Insert particles uniformly in to a slab oriented along three directions



Voronoi construction to determine relative volume



Scale with
Gaussian profile
in perp. dirrection



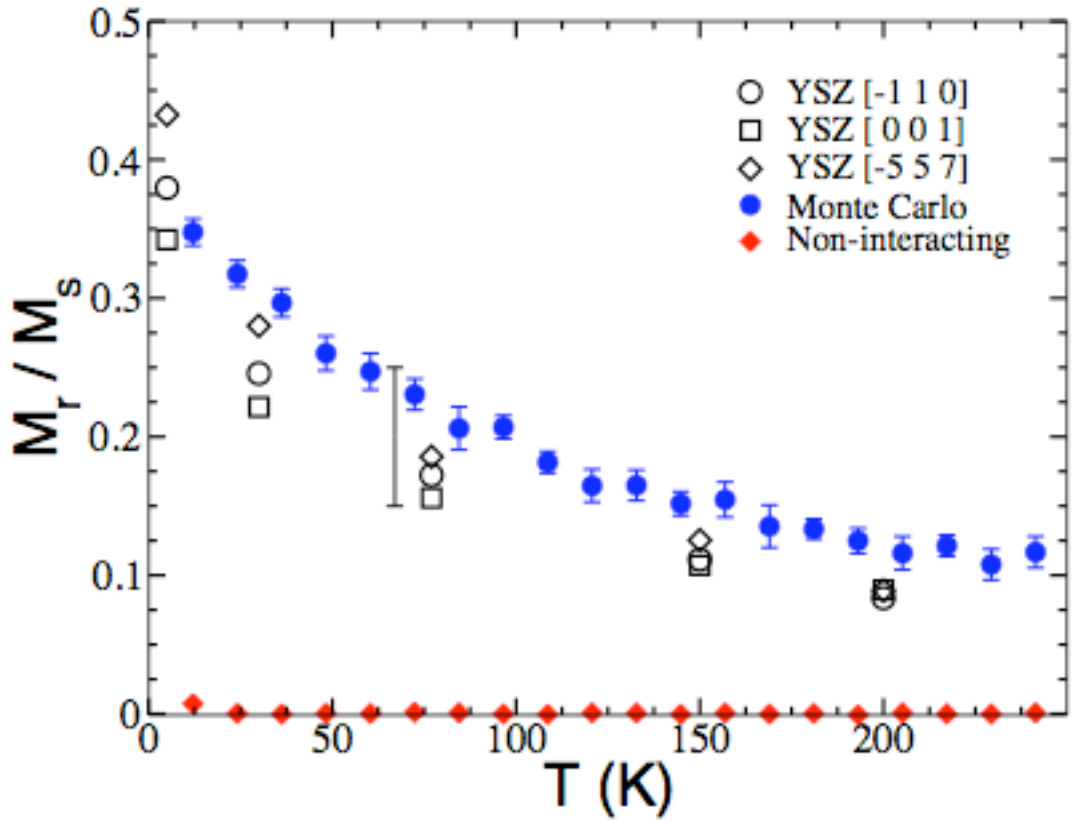
Hamiltonian (no fitting parameters)

$$H = -\frac{1}{2}\sum_{i \neq j} \vec{m}_i \left(\frac{3\hat{r}_{ij}\hat{r}_{ij} - \hat{\hat{1}}}{\left|\vec{r}_{ij}\right|^3} \right) \vec{m}_j +$$

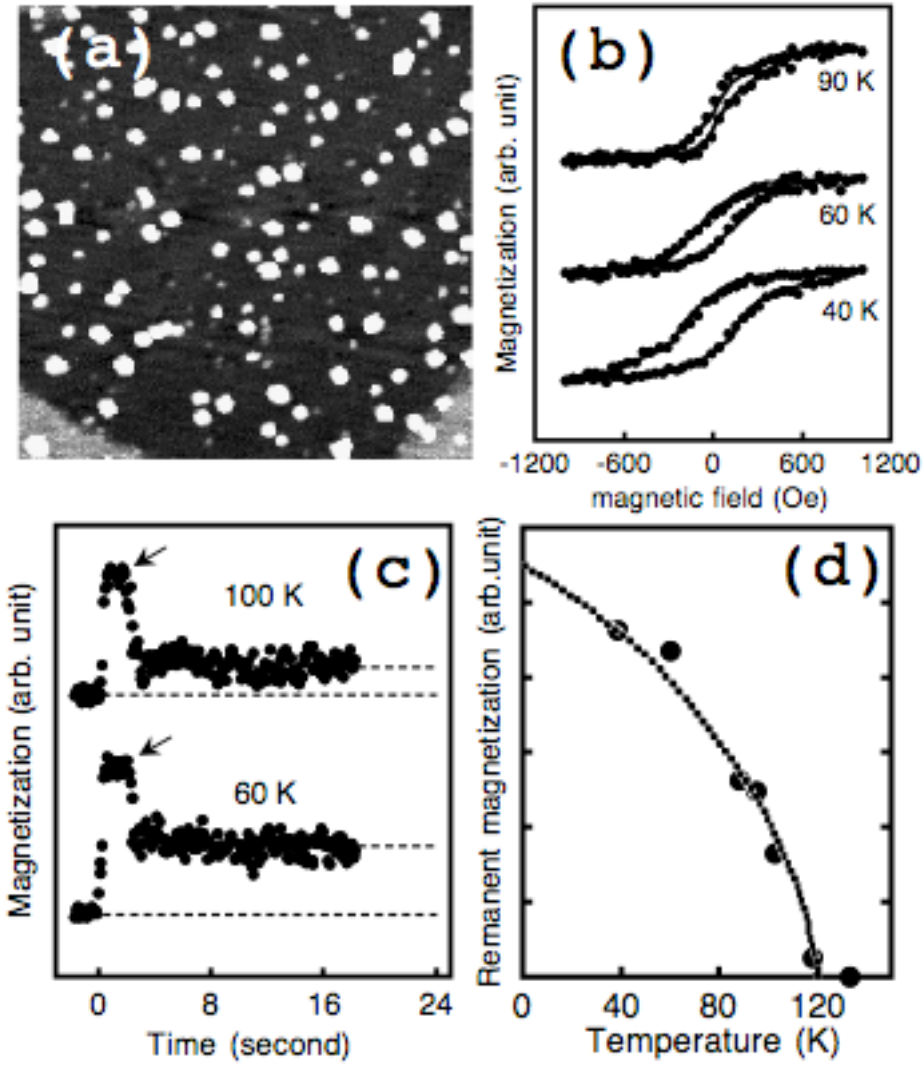
$$K_0 \sum_i V_i \left[(\hat{K}_1^i.\hat{m})^2 (\hat{K}_2^i.\hat{m})^2 + (\hat{K}_2^i.\hat{m})^2 (\hat{K}_3^i.\hat{m})^2 + (\hat{K}_3^i.\hat{m})^2 (\hat{K}_1^i.\hat{m})^2 \right]$$

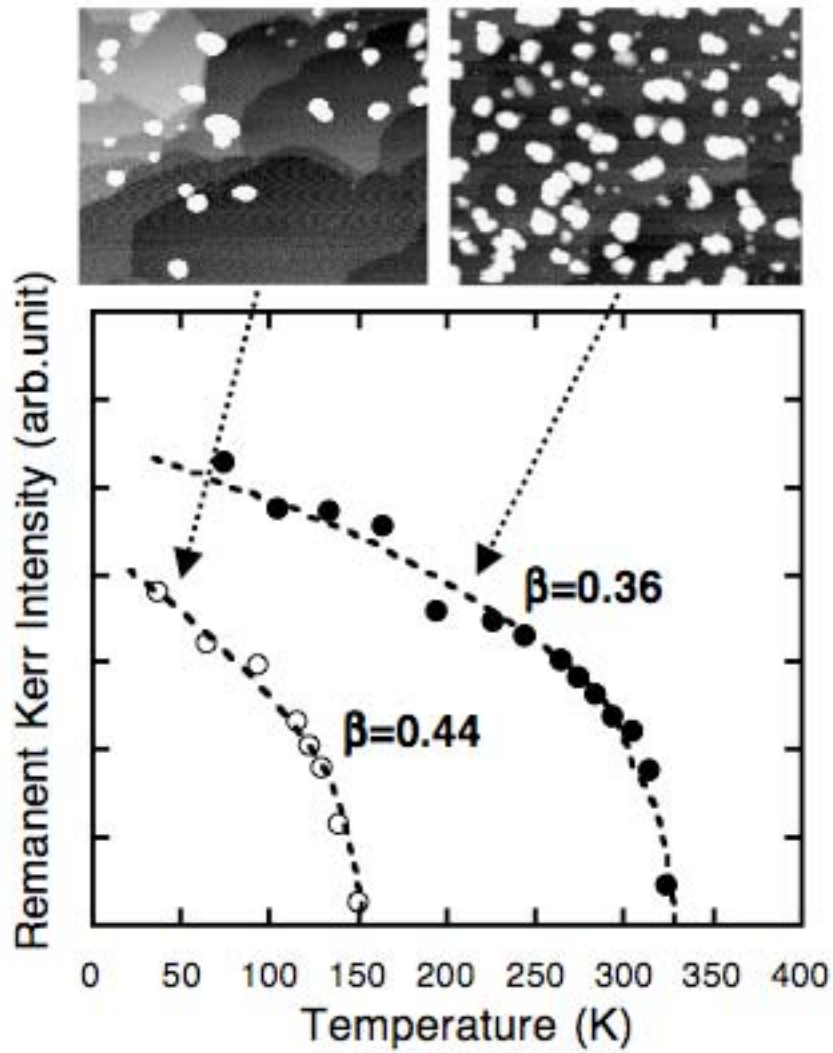
Bulk BCC Fe

Temperature dependence of remnant magnetization

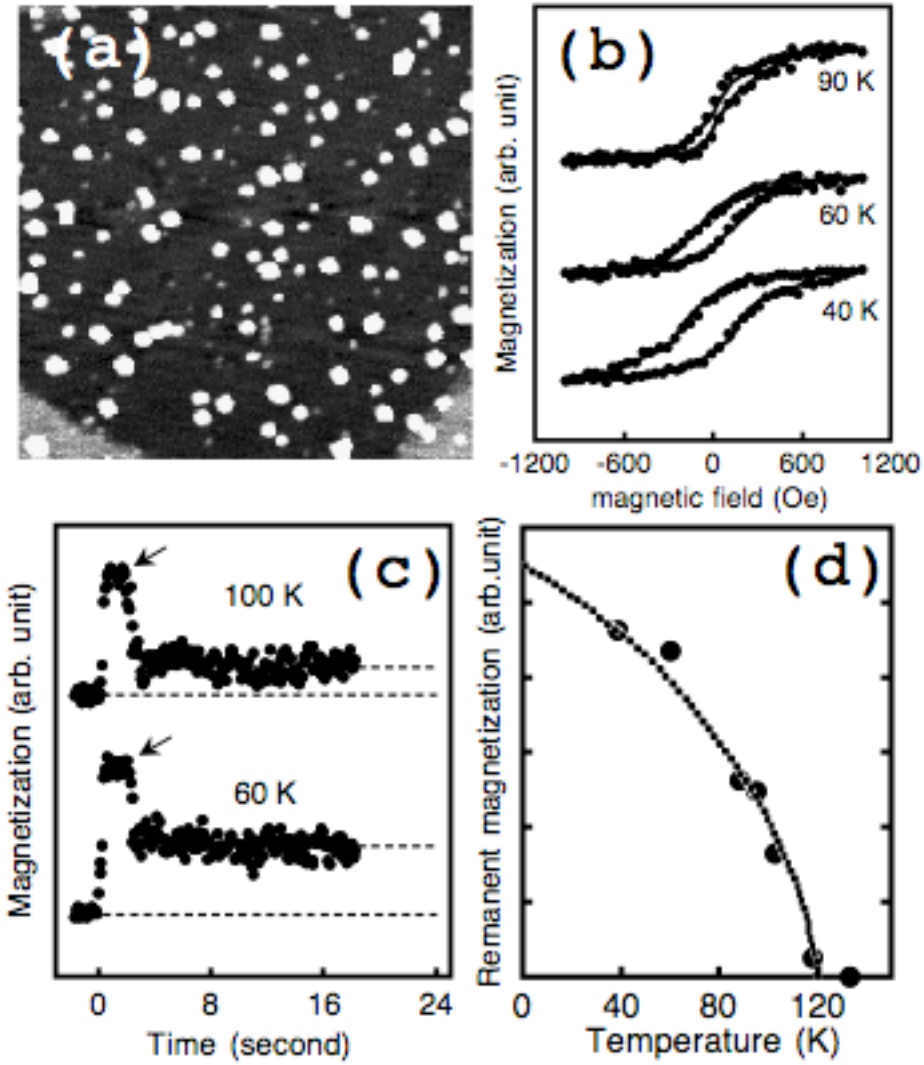


Fe nano-particles on Cu (111)





Constructing the model in this case

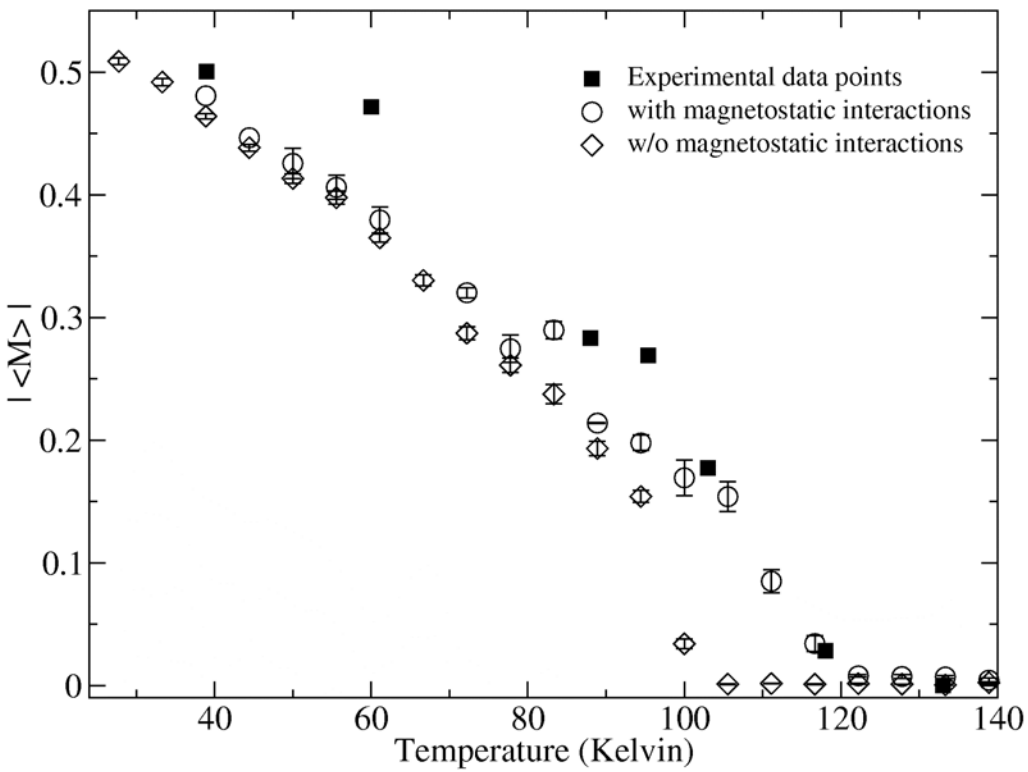


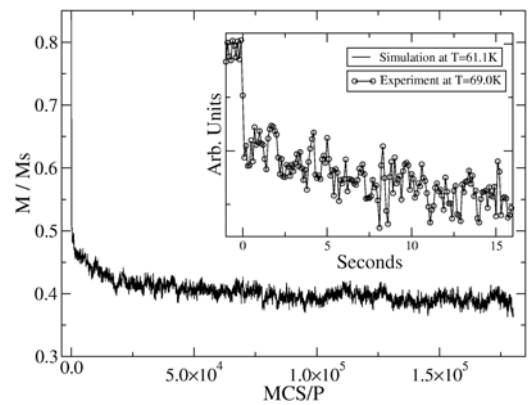
- **Positions and sizes known from experiment**
- **Hamiltonian**

$$H = -\frac{1}{2}\sum_{i \neq j} \vec{m}_i \left(\frac{3\hat{r}_{ij}\hat{r}_{ij} - \hat{\hat{1}}}{\left|\vec{r}_{ij}\right|^3} \right) \vec{m}_j + K \sum_i V_i \cos^2 \vartheta_i$$

- **Uniaxial anisotropy with only free parameter *K***
- **Monte Carlo simulations starting from ordered state**

Monte Carlo Simulations



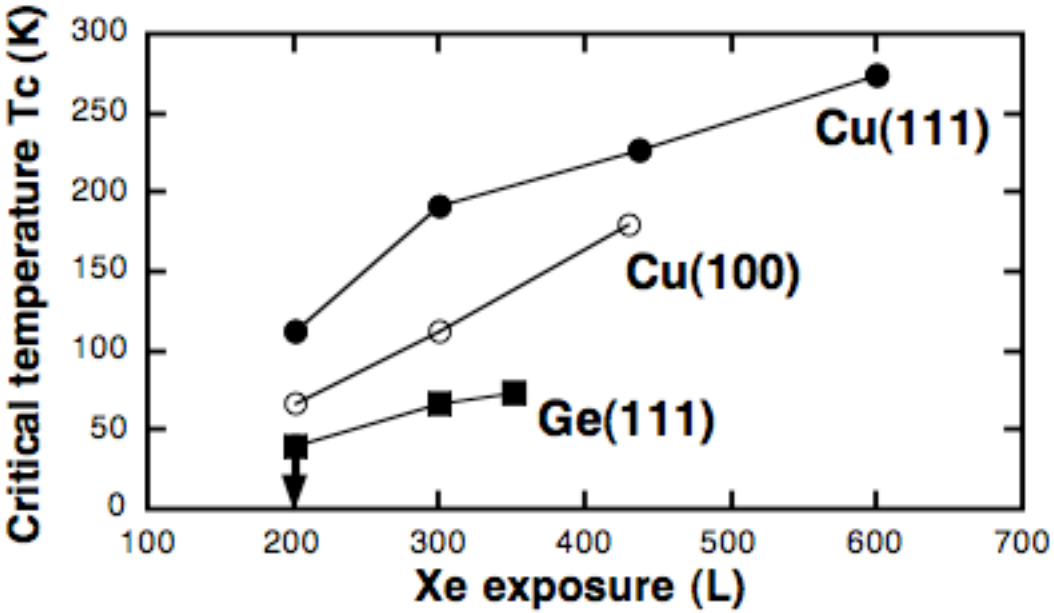


- **Magnetostatic interaction play minor role**
- **Need to increase anisotropy by order of magnitude compare to bulk bcc Fe (?)**
- **But particles are hemispherical**
  - **High anisotropy is hard to justify**

Are we missing something in the model?

Alternative mechanism

- **Cu (111) has a well known surface state**
- **RKKY like interaction between Fe nanoparticles**
  - **2D electron gas, $1/r^2$ decay for atoms**
- **Check hypothesis by changing substrates**



Pierce et. al., Phys. Rev. Lett., (May 2004)

Spin Waves in Paramagnetic Iron

- **Questions: can non-diffusive spin waves exist in paramagnets?**
- **Inelastic Neutron scattering experiments:**
  - **YES: Lynn, PRB (75); Mook and Lynn, JAP (75);**
  - **NO: Collins et al. PR (69); Wicksted et. al. PRB (84);**
- **Theory:**
  - **Possible with short range order postulated: Horeman et al. PRB (1977)**
  - **Only diffusive spin waves: Hubbard PRB (79,81); Morva (91)**
  - **No spin waves with early spin dynamics simulations: Shartry PRL (84)**

Construct a model for this problem

- **3D classical Heisenberg model for BCC lattice**
- **Solve equation of motion for spin system**

$$\frac{d\mathbf{S_r}}{dt} = \mathbf{H}_{eff} \times \mathbf{S_r} \qquad \mathbf{H}_{eff} \equiv -\sum_{\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'} \mathbf{S_{r'}}$$

J_1=18.2 **meV;** ***J_2=10.3*** **meV;** ***J_3=-0.8*** **meV;** ***J_4=1.2*** **meV (*ab initio* calculation)**

- **Calculate spin-spin correlation function**

$$C^k(\mathbf{r}-\mathbf{r}',t) = \langle {S_\mathbf{r}}^k(t) {S_{\mathbf{r}'}}^k(0)\rangle - \langle {S_\mathbf{r}}^k(t)\rangle\langle {S_{\mathbf{r}'}}^k(0)\rangle$$

$$k = x, y, z$$

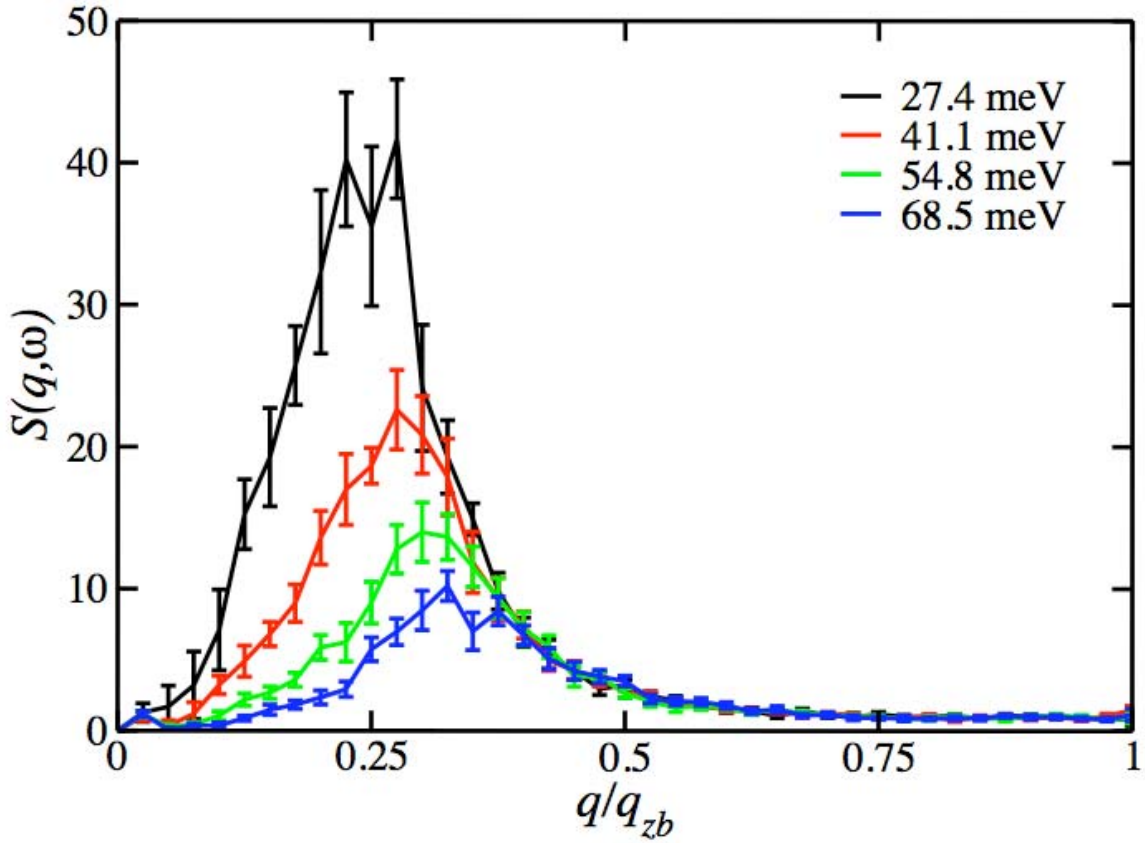
and dynamics structure factor

$$S^k(\mathbf{q},\omega) = \sum_{\mathbf{r},\mathbf{r}'} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_{-\infty}^{+\infty} e^{i\omega t} C^k(\mathbf{r}-\mathbf{r}',t) \frac{dt}{\sqrt{2\pi}}$$

- **Computational challenge:**
  - **Large systems (40x40x40 lattice = 128K spins)**
  - **Long time scale integration: Trotter dynamics**
  - **Good statistics: average over many runs**

(generate initial state with Metropolis MC)

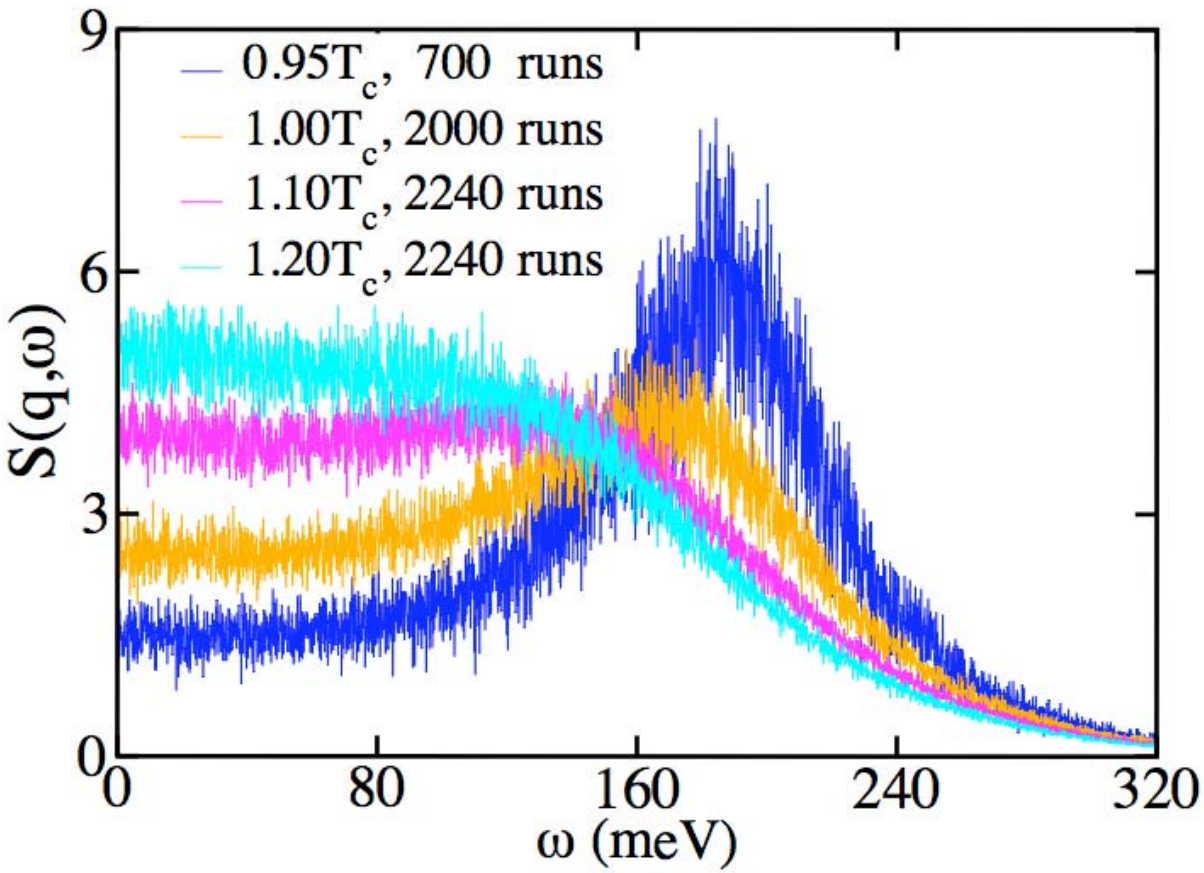
Constant Energy Scans:



Constant E scan along $(q,q,0)$

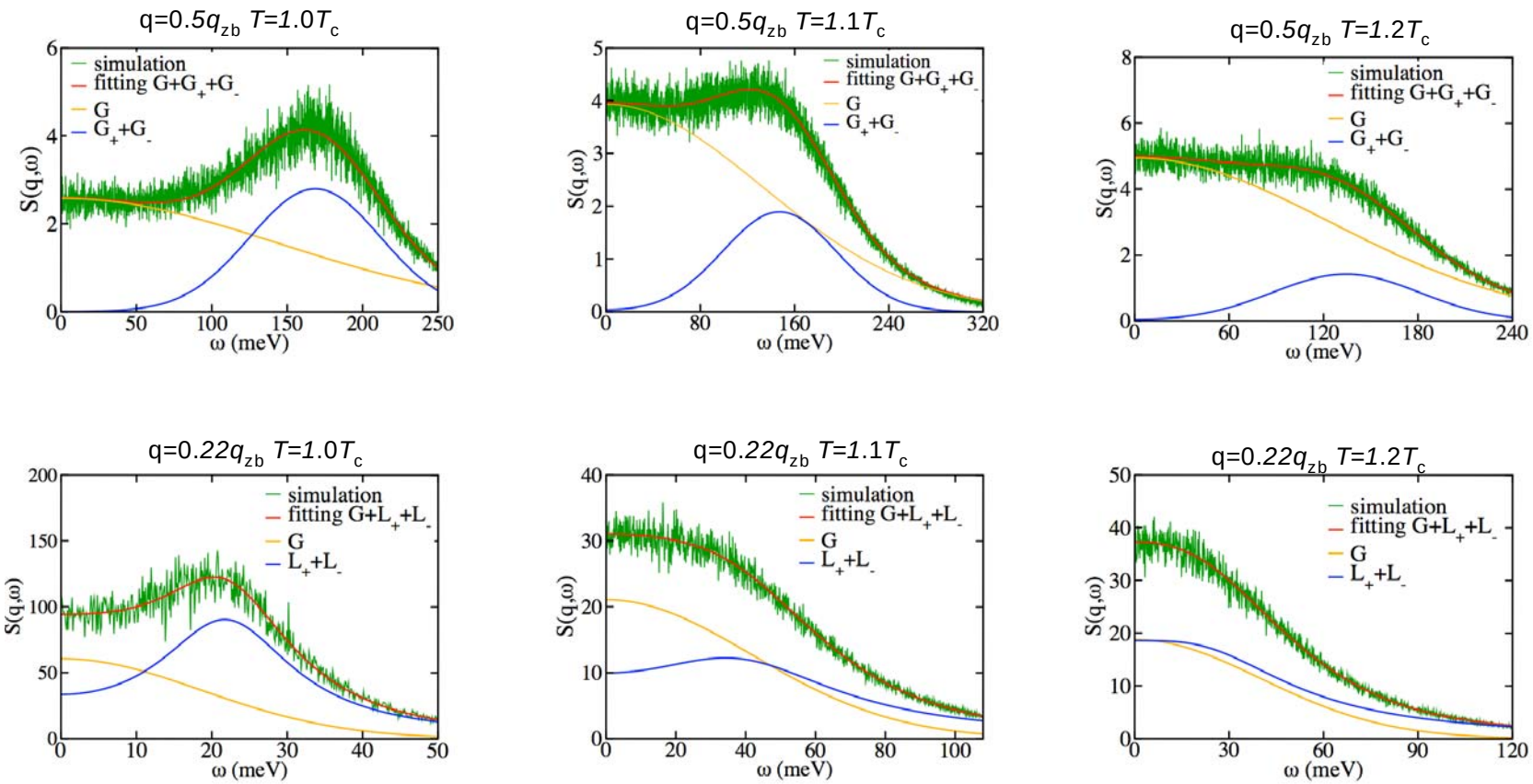
Constant *q* Scan:

$$\boldsymbol{q}=\pi/a(1,0,0)$$

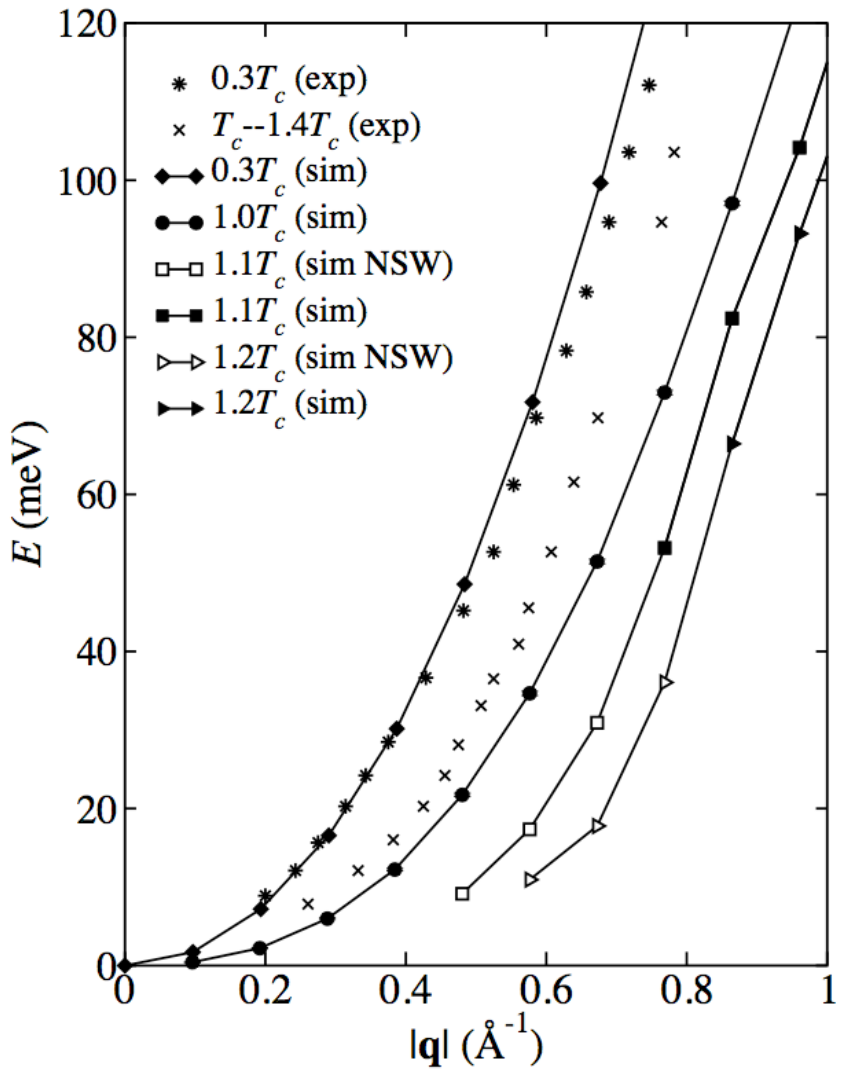


Analyzing the Structure Factor

$$S(\mathbf{q},\omega) = G + G_+ + G_- \qquad S(\mathbf{q},\omega) = G + L_+ + L_-$$



Dispersion below, at, and above T_c



- **Non-diffusive spin waves only defined for large *q* vectors**
  - **Consistent with magnetic short range order**
- **Dispersion above and below T_c similar**
- **Traveling spin waves in paramagnetic iron definitely exist!**

Extensible "Heisenberg" Model

$$E\left[\left\{\vec{m}_i\right\}\right] = -\sum_{i \neq j} J_{ij} \vec{s}_i \vec{s}_j - \frac{1}{2} \sum_{i \neq j} \vec{m}_i \frac{3\hat{r}_{ij}\hat{r}_{ij} - \hat{\hat{1}}}{\left|\vec{r}_{ij}\right|^3} \vec{m}_j + \sum_i K_i \sin\theta_i + \cdots$$

- **Flexibly add / remove energy terms**
- **Efficient algorithms to evaluate energy terms**
  - **Long range interactions (FFT, FMM, Ewald)**
- **Various types of Monte Carlo sampling schemes**
- **Spin dynamics simulations**
  - **Regular spin dynamics; Trotter dynamics; Stochastic dynamics**

Currently Planned Extensions

- **Spin Fermion Models**
  - **Apps: Manganites, Dilute Magnetic Semiconductors**

$$H = -t \sum_{<ij>\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - J_H \sum_{i\alpha\beta} c_{i\alpha}^{\dagger} c_{i\beta} \vec{S}_i \cdot \vec{\tau}_{\alpha,\beta}$$

  - **Based on realistic band structure (LDA, SIC-LSD)**
- **Free energy surface of magnetic nanoparticles**
  - **Apps: FePt, CoPt, magnetic data storage**
  - **Challenge: simple spin models fail (1/3 at. @ surface)**

$$E\left[\{\vec{m}_i\}\right] \rightarrow E\left[n(\vec{r}), \vec{m}(\vec{r})\right]$$

  - **Energy functional based on Local Spin Density Approximation to Density Functional Theory**

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Implementation: The *Ψ-Mag* Toolkit

- **C++ library for computational magnetism and serves as a prototype for a more general library for computational materials science.**
  - **New effort: expand *Ψ-Mag* for molecular simulations**

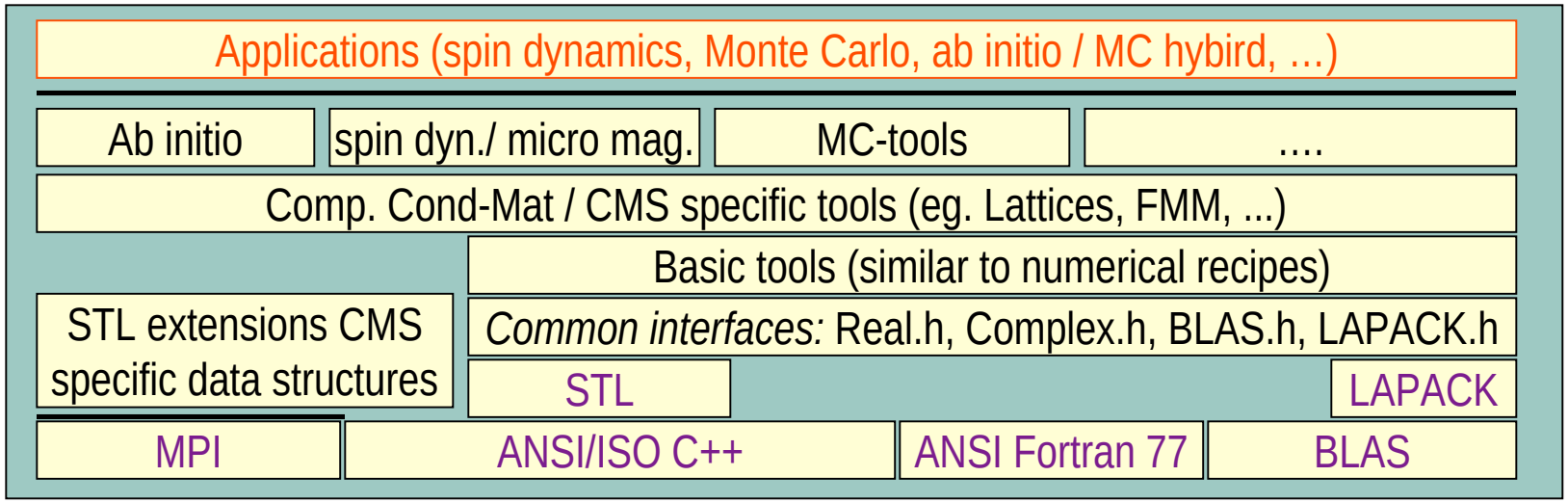
- **Design is modeled and inspired by the generic programming techniques of the C++ standard template library (STL).**

Language: C++ and the STL

- **C++ programming language:**
  - **Object oriented "extension" of C**
    - →*Can be as efficient at C*
  - **Support of *templates* (replacement of pre-processor)**
    - →*Templates allow for compile time polymorphism*
- **Standard Template Library (STL)**
  - **Generic algorithms and data structures (lists, sort, …)**
  - **Designed for extensibility: "to use STL is to extend it"**
  - **Algorithms are decoupled from containers**
  - **Extensible and customizable without inheritance**
  - **Abstractions based on compile time polymorphism**
- **C++ (and STL) exist on HPC just like C & Fortran**

Ψ-Mag Toolkit: an extension of STL

- **No claim for completeness:**
  - **Implement carefully what is needed**
  - **Extensible design makes adding tools rather simple**
- **Layered software structure with minimal interdependence**
  - **no horizontal dependence**
  - **Individual classes are simple**

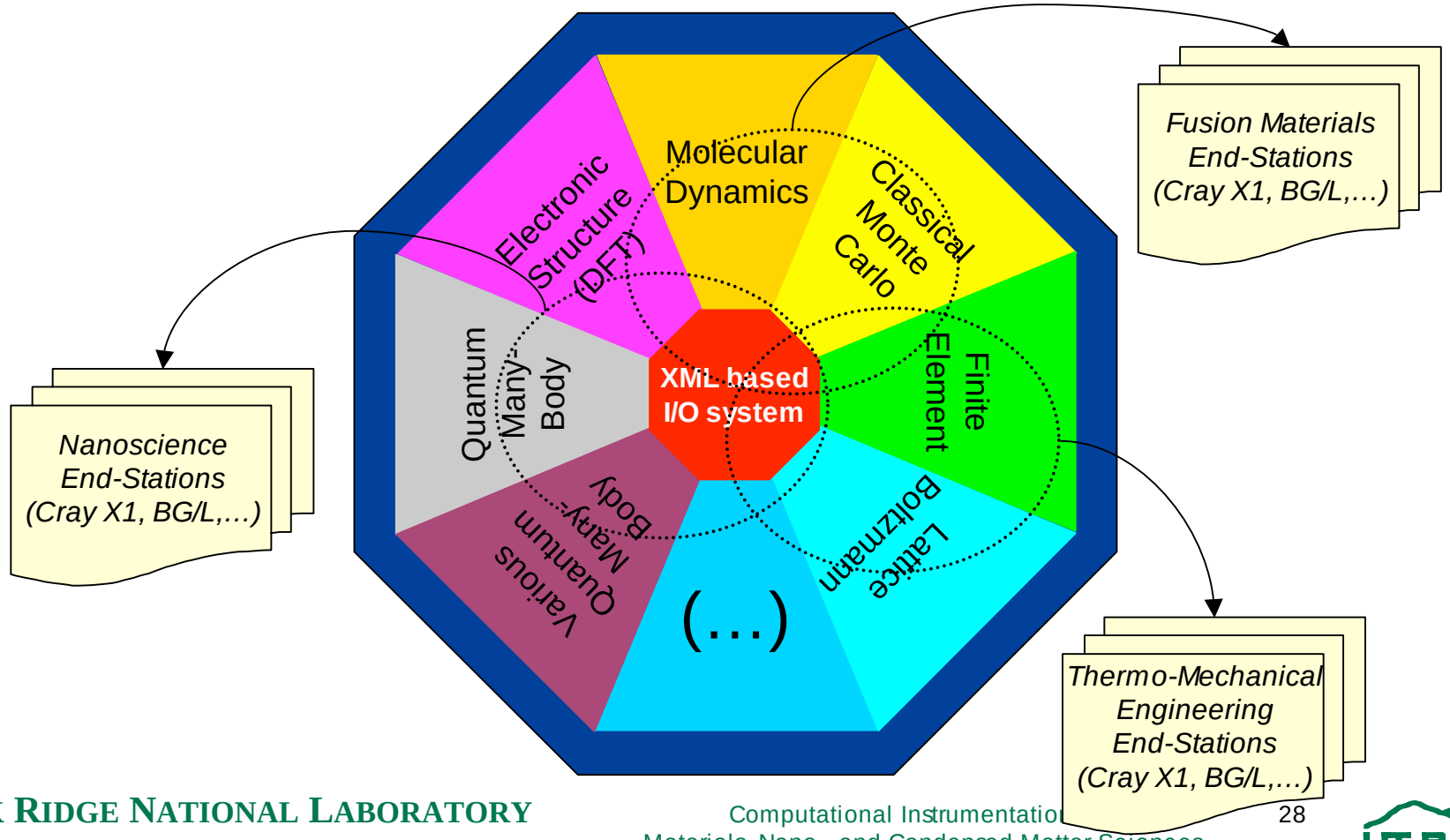


- **Applications using *Ψ-Mag*:**
  - **Can access all layers directly**
  - **Small and therefore flexible / maintainable**

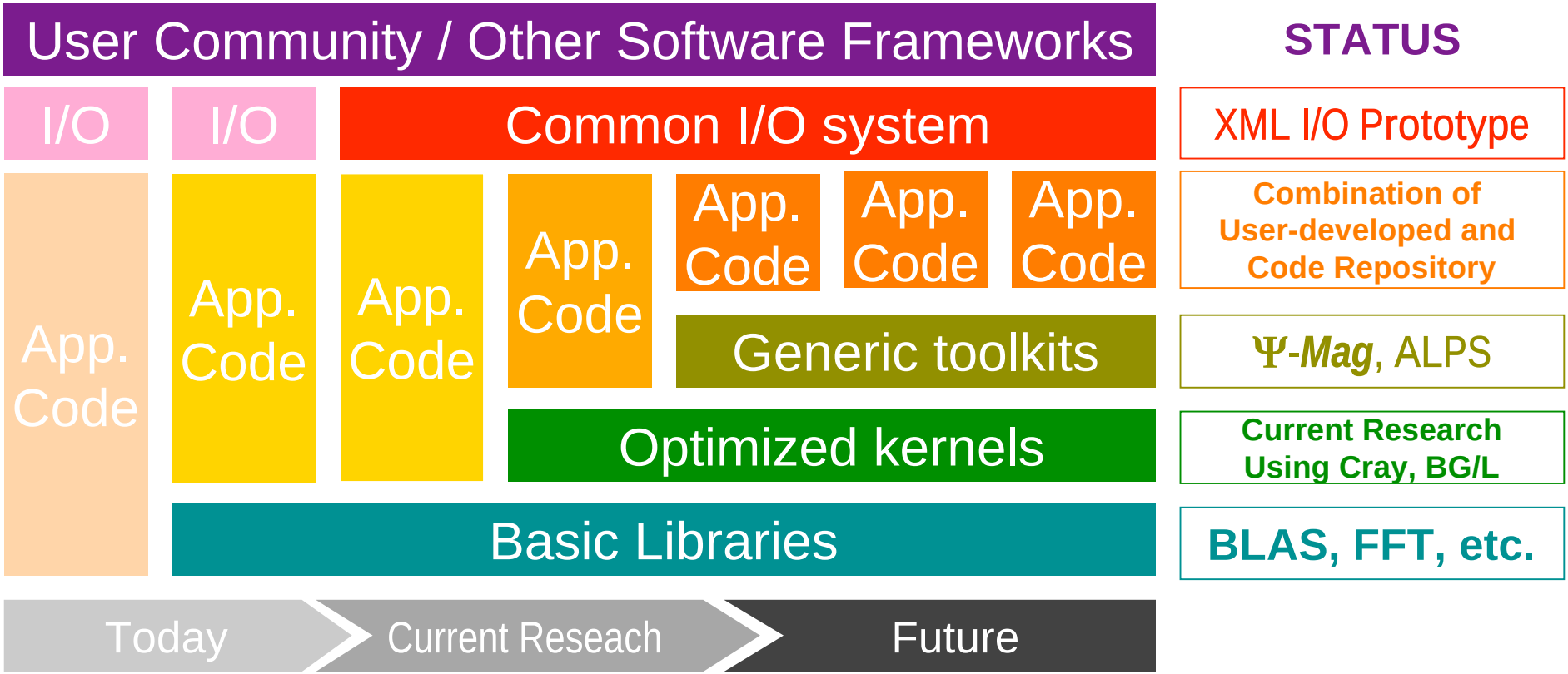
- **New site approximately end of April 2005: http://psimag.org**

Code Repository built ...

- **around common I/O system**
  - **emphasis is on user**
- **with community and from existing codes**



A Meaningful Evolution of Software?



- **Reduce size of application code**
- **Improve usability of codes**
- **Enhance productivity / creativity**

- **Optimize performance / efficiency**
- **Simplify user access to machines**
- **Prioritization of resources**

Lots of Opportunities in Nanoscience at ORNL:

Center for Nanophase Materials Sciences

Nanomateirals Theory Institute

Inaugural CNMS User Meting

May 23-25, 2005

Registration Now Open

http://www.cnms.ornl.gov/

Acknowledgments

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