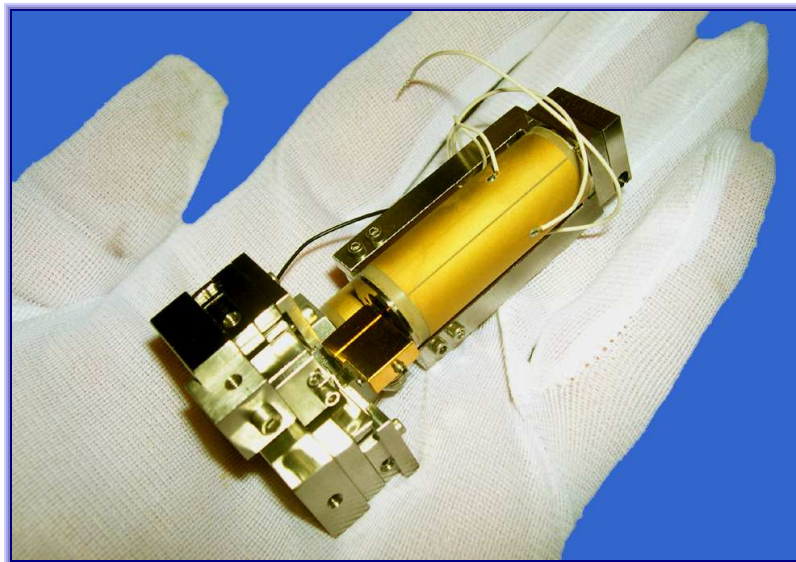


# PROGRAM FOR ACHIEVING SINGLE NUCLEAR SPIN DETECTION

A UW QUANTUM SYSTEM ENGINEERING WHITE PAPER



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**Abstract:** This white paper discusses the technical feasibility of comprehensive molecular imaging, and what such a capability might imply. Care has been taken to make this material accessible to nonspecialists, yet the discussion is reasonably rigorous. The following questions are addressed:

- (1) What is a reasonable technical path to single-nuclear-spin detection?
- (2) What are appropriate performance metrics and technical milestones?
- (3) When might this technology reasonably be ready?
- (4) What tasks could this technology accomplish?
- (5) How can it help in the Global War on Terrorism?

Section I provides a one-page summary of answers to these questions. Detailed answers are given in the body (Sections II–VI).

## I MRFM Questions and Answers

The year 2004 was a breakthrough year for magnetic resonance force microscopy (MRFM): the detection of a single electron spin by Dan Rugar's IBM group culminated a twelve-year effort during which MRFM sensitivity has improved by 140 dB. This equates to a doubling of MRFM sensitivity every 3.1 months for twelve years—a rate of progress unequalled by any sensor technology in history.

### **What is a reasonable technical path to single-nuclear-spin detection?**

The natural technical path is by continued development and testing of smaller, colder, quieter MRFM devices.

### **What are appropriate performance metrics and technical milestones?**

A natural metric is the single-spin *channel capacity*, defined as the bits-per-second of imaging information received from each spin. A natural milestone is 0.1 bits-per-second, which is a threshold rate at which single-spin detection becomes feasible.

### **When might this technology reasonably be ready?**

Atomic-resolution imaging will become feasible in  $\sim 2010$  if present progress is sustained. Sustaining this progress will require three coordinated efforts:

- (1) fabricating the next generation of MRFM devices: smaller, colder, and quieter,
- (2) testing these devices in real-world imaging environments, and
- (3) synthesizing reliable engineering principles from the emerging nanoscale physics.

The purpose of this white paper is to help build a community to undertake these efforts.

### **What tasks could this technology accomplish?**

To the extent that maturing MRFM technologies can approach the quantum limits to channel capacity, tabletop-scale devices will observe hundreds of atomic coordinates per second. A cluster of several hundred such devices, deployed like the clusters of sequencers in the Human Genome Project, would observe in excess of  $10^{12}$  coordinates per year.

Archiving, interpreting, and sharing this rich flow of structural data would comprise the largest scientific project in history. As pay-off, the unifying context of the project would amplify the value of a broad spectrum of atomic-scale imaging projects relating to (*e.g.*) materials science, nanoscale electronics, quantum physics, biology, and medicine.

### **How can it help in the Global War on Terrorism?**

Recent defense analyses have concluded that wisely-mobilized resources provide an essential foundation for victory in the struggle against terror. From a resource-centric point of view, the strategic roles of MRFM technology are:

- (1) **TELESCOPES FOR CHEMICAL SPACE** As a scientific resource, atomic-scale imaging will provide observational access to the “chemical space” of nanoscale structures.
- (2) **RADAR FOR MOLECULES** As a defense resource, atomic-scale imaging will provide detailed intelligence of natural and/or engineered threats emerging in chemical space.
- (3) **FOUNDATIONS FOR NEW TOOLS, PRODUCTS, AND MARKETS** As an economic resource, atomic-scale imaging will open new commercial frontiers of unbounded scope.

## II About This White Paper

It is the practice of our Quantum System Engineering (QSE) Group to post our proposals on our [web site](#) as white papers.<sup>a</sup> This public sharing is one of the great pleasures and rewards of teaching. Also, the white papers discipline our thinking, by exposing it to public review and criticism, and they help us recruit students and collaborators.

**Syllabus and Lessons Learned** This white paper strives to integrate well-known, well-tested ideas into a unified program of quantum system engineering (QSE). Purely technical citations are confined to the body of the white paper. To provide context, this section gives a syllabus of non-technical sources and the lessons we learned from them.

**Lessons from Engineering and Science** Guerlac’s *Radar in World War II* [37] is an indispensable resource, as is Rasmussen’s *Making a Machine Instrumental: RCA and the Wartime Origins of Biological Electron Microscopy in America, 1940-1945* [78], and Collins’ *Gravity’s Shadow* [22]. In the early post-war period, the microscopy-related research of Pauling [74], von Neumann [102], and Feynman [33] is inspirational yet sobering,<sup>b</sup> as is Schwinger’s radar-related research [37, 68, 84] and Bardeen’s applied physics research at Xerox [47]. Murray and Millet’s *Military Innovation in the Interwar Period* gives an overview of modern military scholarship; the chapters by Beyerchen [4], Murray [70], and Millet [69] are particularly valuable. The pivotal role of new technologies in accessing the resources of “chemical space” has recently been emphasized [1, 28, 56, 62].

**Lessons from Business** We have borrowed many ideas from Rickover, Boyd, Toyodo, Shingō, and Ōno. We embrace Rickover’s strategy of development-in-parallel [5, 32]. We embrace Boyd’s concepts of graphical performance metrics [3, 7, 23, 46, 79]. Footnotes acknowledge the insights of Shingō [86] and Ōno [72], and in particular, we embrace Ōno’s insight “What is important is having all the elements together as a system [that is] practiced every day in a very consistent manner” [61, page xv].

**Lessons from Defense** Our primary defense readings are the Army’s Field Manual (Interim) FMI 3-07.22 *Counterinsurgency Operations* [26], and the National Intelligence Council’s 2020 Project: *Mapping the Global Future* [71]. The word “resource” appears 112 times in these two analyses, and it generally plays a crucial role. In focussing on resources, these analyses mesh reasonably seamlessly with the DoD’s classic *Chief of Staff* [103] and with Jared Diamond’s recent *Collapse: How Societies Choose to Fail or Succeed* [27].

**Uniting the Lessons** Our students learn from this syllabus that MRFM development is as exciting and potentially as rewarding as any development effort in history. They learn sobering lessons too: technology development is difficult, success is not guaranteed, teambuilding is challenging, and persistence is an absolute requirement.

In uniting these lessons, our greatest debt is to the [thought and example of Marshall](#) [24], who showed that wisely-mobilized resources—both material and spiritual—provide solid foundations for freedom and democracy, and powerful engines for economic prosperity. We believe the objectives of Marshall’s Nobel Peace Prize lecture [67] can be achieved in this century, and we hope and plan that our work will help achieve them.

<sup>a</sup>The white papers have added material for non-specialists, in the form of footnotes.

<sup>b</sup>See <http://courses.washington.edu/goodall/MRFM/historical.background.html>.

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### III The Proposed Program

**Program Goal** This program [73] will conduct basic research leading to a proof-of-concept magnetic resonance force microscope (MRFM) that demonstrates *in situ* detection of individual nuclear magnetic moments and three-dimensional mapping with atomic resolution.

**Approach** The program will design and fabricate MRFM devices that can detect single nuclear spins. Specifically, these devices will achieve a single-spin channel capacity of 0.1 bits-per-second, *i.e.*, they will acquire one bit of imaging information in ten seconds of nuclear spin observation.<sup>1</sup> A series of imaging trials will generate a validated understanding of spin physics and noise mechanisms; this will determine the best design path for achieving the program's performance goals. A complete proof-of-concept system will be built, including magnetic tips, cantilevers, sensors, sample scanners, cryogenics, digital controllers, and signal-processing software.

**Milestones and Timeline** The three-year base-period milestones will be:

- (1) Fabricate a development platform.
- (2) Fabricate acoustic and megahertz cantilevers for single-nucleon detection.
- (3) Conduct 3D imaging trials at a resolution of 100, 10, and 1 nanometers.
- (4) Extract validated spin physics, noise budgets, and quantum design rules.
- (5) Finalize the design and operating methods for single-nuclear-spin detection.

The two-year option milestones will be:

- (6) Reduce technical noise to within 30 dB of the quantum capacity limit.
- (7) Demonstrate single-nuclear-spin detection in a practical imaging context.

<sup>1</sup>Recent IBM experiments show single-spin detection is feasible at this threshold capacity.

**Deliverables** The deliverables are a validated science and engineering knowledge-base that suffices for single nuclear spin detection, and a design and laboratory prototype of a field-deployable imaging unit.

**Team and Management Plan** This program is a joint effort of the University of Washington (John Sidles and Joe Garbini), Cornell University (John Marohn), and the University of Michigan (Al Hero), with the Army Research Lab (ARL) (Doran Smith) and IBM (Dan Rugar) in consultative roles.

The team was selected for outstanding multidisciplinary expertise in theoretical and experimental physics, mechatronic engineering, signal processing, nanofabrication, chemistry, and defense research.

Members of this team invented MRFM and during the years 1992–2004 improved its capacity by  $\sim 140$  dB. This equates to a doubling of MRFM capacity every 3.1 months for twelve years—a rate unequalled by any sensor technology in history.

**Anticipated Outcome** Achieving the program goal will open the door to deployable MRFM devices with comprehensive atomic-scale 3D imaging capability.

**Impact on DoD Capabilities** Comprehensive atomic-scale microscopy will exert a transformational impact on DoD capabilities in materials science, multifunctional materials, nano-electronics, and biodefense.

#### Scientific and Technical Impact

Atomic-scale microscopy will be an enabling technology for multidisciplinary science and engineering at the intersection of chemistry, physics, nanoelectronics, and biology.

**Educational Impact** The knowledge-base required for practical single-nuclear spin microscopy will comprise a new engineering discipline: *quantum system engineering*. This new discipline will stimulate both US engineering and US industry.

## IV Statement of Work

### IV.1 Scope and Objectives of the Effort

This program [73] will conduct basic research leading to a proof-of-concept magnetic resonance force microscope (MRFM) that demonstrates *in situ* detection of individual nuclear magnetic moments, and three-dimensional mapping with atomic resolution.<sup>2,3</sup>

### IV.2 Specific Research to Be Performed

TASKS RELATING TO DESIGN & APPARATUS		
1.1	<i>Scanner modifications</i>	Refit for Larmor and acoustic cantilevers.
1.2	<i>Cantilever/Tip fabrication</i>	Fabricate acoustic and Larmor cantilevers
1.3	<i>Interferometer improvement</i>	Focused fiber-optic interferometer
1.4	<i>Technical noise mitigation</i>	Mitigate close-approach sample noises
1.5	<i>Advanced refrigerator design</i>	Analyze/design vibration requirements
1.6	<i>Refrigerator install/test</i>	Convert UW scanner advanced refrigeration
TASKS RELATING TO EXPERIMENTS		
2.1	<i>Technical noise studies</i>	Survey non-thermal noise mechanisms
2.2	<i>Imaging trials</i>	Image at 100, 20, and 1 nm resolution.
2.3	<i>Acoustic iOSCAR</i>	Acoustic single-nucleon detection trials
2.4	<i>Larmor iOSCAR</i>	Larmor single-nucleon detection trials
TASKS RELATING TO THEORY AND ANALYSIS		
3.1	<i>Single-nucleon physics</i>	Investigate single-spin detection physics
3.2	<i>Multi-nucleon analysis</i>	Investigate multiple-spin detection physics
3.3	<i>Technical noise analysis</i>	Technical noise analysis and mitigation
TASKS RELATING TO SIGNAL PROCESSING		
4.1	<i>Signal processing</i>	Advanced noise analysis techniques
4.2	<i>DSP and control</i>	Closed-loop system emulation and control
4.3	<i>Image reconstruction</i>	Optimize imaging information rate

Table 1: Table of research tasks to be performed

## V Technical Approach

### V.1 The Elements of Magnetic Resonance Force Microscopy

**How MRFM Works** The essential elements of an MRFM imaging device are shown in Figure 1. MRFM combines scanning probe microscopy with magnetic resonance imaging. As

<sup>2</sup>The footnotes of this white paper quote extensively from an AFOSR-supported study entitled *The Toyota Way* [61, p. XIX]. However, our thinking owes an even greater debt to the official DoD history entitled *Chief of Staff: Prewar Plans and Preparations* [103]. See footnote 28 on page 22 for further comments.

<sup>3</sup>Toyota’s founder Kiichiro Toyoda said [61, p. 18] “Everyone should tackle some great project at least once in their life. I devoted most of my life to making new kinds of looms. Now it is your turn. You should make an effort to complete something that will benefit society.” This is one of two chief reasons our QSE Group admires the Toyota Way. The other reason is Toyota’s philosophy of “unrelenting pursuit of perfection in every aspect.” After reflecting (*hansei*) on this goal, we regard it as the central organizing principle of quantum system engineering (see footnote 27 on page 21).

in magnetic resonance imaging, sample spins couple resonantly to an applied radio-frequency field if and only if they are located within a resonant slice.

In MRFM this resonant slice is generated by the magnetic tip of a force microscope cantilever. The spatial gradient of the magnetic field is very large, such that spin precession is resonant with the applied radio-frequency field only within a very thin slice—a slice whose thickness is comparable to atomic dimensions.

The presence of magnetic resonance is detected mechanically, via the magnetic force exerted between the spin and the sample. For a single nuclear spin this force is extremely small, of order  $10^{-18}$  N, or one attoNewton (abbreviated aN). Yet even this small force is enough to excite the force microscope cantilever, whose motion is typically detected by an optical interferometer.

By scanning the cantilever over the surface, and recording the consequent MRFM signal, the three-dimensional distribution of spins within the sample can be determined, by reconstruction methods similar to those in conventional magnetic resonance imaging.

**MRFM Performance Metrics** In imaging with single-spin resolution, it is natural to regard each spin as a transmitter that sends information to the outside world via the cantilever. Because the cantilever is noisy, there is a limit to the bits-per-second that an individual spin can transmit. This limiting data-rate is well-known to signal processing engineers, and is called the *channel capacity* [34, 64].<sup>4</sup>

**MRFM’s Exponential Progress** MRFM’s capacity has improved exponentially during the twelve years since its invention: the single-nuclear-spin capacity has increased by 140 dB, *i.e.*, by fourteen orders of magnitude. This corresponds to a doubling of capacity every 3.1 months, sustained for 46 consecutive doublings. Our goal is to sustain this same exponential rate of improvement for the five years of the program, which will suffice to achieve the main objective of Program Topic #6: the detection of a single nuclear spin [73].<sup>5</sup>

## V.2 Summary of our Team’s Assets and Capabilities

Our Program Team has fabricated and operated several generations of MRFM devices, and we are, by a considerable margin, the most experienced university-based MRFM team in the world.<sup>6</sup> The proposed single-nuclear-spin program effort is the logical next step in our

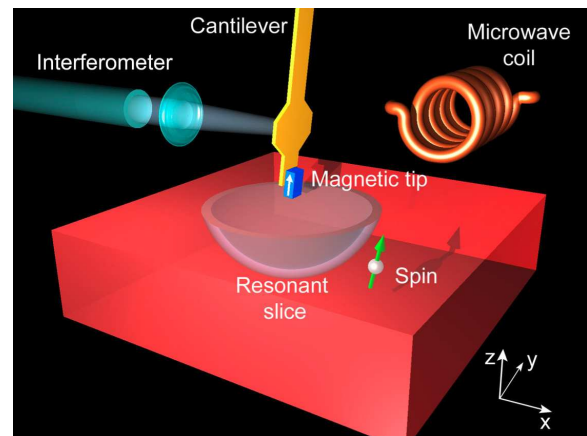


Figure 1 Elements of an MRFM imaging device, adapted from Rugar *et al.* [81].

<sup>4</sup>This white paper’s emphasis on capacity-based performance metrics (Sections V.5–7) borrows heavily from John Boyd’s techniques for energy-maneuverability analysis [23, 46]. Boyd’s specific excess power (SEP) metric played a pivotal role in evolving aircraft design from a largely intuitive activity [48] into a more rigorously quantitative one [3, 7, 79]. The graphical tools of Table 3 on page 16 are directly inspired by Boyd’s work: see footnote 23 on page 18 for details.

<sup>5</sup>Adapted from *The Toyota Way* [61, p. 24]: “The Japanese term for continuous improvements is *kaizen*, and is the process of making incremental improvements, no matter how small. . . *Kaizen* is a total philosophy that strives for perfection and sustains the [Toyota production system] on a daily basis.”

<sup>6</sup>Adapted from *The Toyota Way* [61, p. 39]: “Develop exceptional people and teams who follow your company’s philosophy.”

long-term development of MRFM technology. Key MRFM subsystems and their status are reviewed in the following paragraphs.<sup>7,8</sup>

### ***Closed-loop 3D MRFM Scanner***

Single-nucleon MRFM experiments will impose unprecedented requirements for tip-sample positioning accuracy and stability on the apparatus. Because positional errors are manifested as an additional source of technical noise, the requirements for both detection experiments and molecular imaging are the same: 3D positioning with resolution comparable to interatomic spacing. In addition, detection and imaging experiments require that positional accuracy must be maintained over hours.<sup>9</sup>



Figure 2 A working 3D MRFM scanner

Joe Garbini is lead mechatronic and control engineer of our team, and his design strategy for the UW MRFM scanner is twofold: careful design of all passive elements, and careful control of all dynamic elements.<sup>10</sup> The scanner shown is presently operating with closed-loop feedback control with long-term 3D accuracy of better than 1 nm.

Profs. Garbini and Sidles have collaborated in MRFM for many years, with a publication record [9–13, 16, 29–31, 35, 82, 87–96, 104] that includes the invention of MRFM [87], coauthorship with Dan Rugar’s IBM group of the first MRFM experiment [82], the first MRFM review article [92], and recently 3D MRFM imaging [16] with 80 nm voxels. Nine graduate-level engineering degrees having thesis topics specifically focussed on MRFM have come out of the UW MRFM Group [14, 17, 20, 50, 51, 53, 63, 75, 83].<sup>11</sup> Profs. Garbini and Sidles are also members of the LIGO Scientific Collaboration (LSC) [96].

<sup>7</sup>Within our QSE Group, the scanner shown in Fig. 2 is called “*Rickover*,” to honor Admiral Hyman Rickover’s historic strategy of developing the reactor and the hull of the the submarine *Nautilus* in parallel, rather than sequentially [5, 32]. Rickover’s development-in-parallel strategy saved years of time, and more importantly, imposed a Toyota-style discipline upon the US nuclear submarine effort that minimized error, reduced risk, and improved efficiency.

<sup>8</sup>Our IBM colleague Dan Rugar is fond of saying “Go into the laboratory and begin by failing as fast as you can.” This echoes the philosophy of Toyota’s Fujio Cho [61, p. 3]: “There are many things one doesn’t understand and therefore, we ask them why don’t you just go ahead and take action, try to do something? You realize how little you know and you face your own failures and you simply can correct those failures and redo it again and at the second trial you realize another mistake or another thing you didn’t like so you can redo it once again. So by constant improvement, or should I say, the improvement based upon action, one can rise to a higher level of practice and knowledge.”

<sup>9</sup>Ichiro Suzuki in *The Toyota Way* [61, p. 42] “Even if the target seems so high as to be unachievable at first glance, if you explain the necessity to all the people involved and insist on it, everyone will become enthusiastic in the spirit of challenge, will work together, and will achieve it.”

<sup>10</sup>Our students know that Prof. Garbini thoroughly embodies the ideal that [61, p. 37] “Leaders thoroughly understand the work, live the philosophy, and teach it to others.” Also from [61, p. 137]: “The biggest challenge [Toyota] faced in training young engineers is to slow them down and get them to stop and reflect on all the alternatives they should consider.” In short, Prof. Garbini is our lead engineer in the Toyota sense.

<sup>11</sup>From *The Toyota Way* [61, p. 250] “Learning is a continuous company-wide process as superiors motivate and train subordinates; as predecessors do the same for successors, and as team members at all levels share knowledge with one another.”

### Advanced Cantilever Fabrication

John Marohn will lead the cantilever and tip development effort. Working at the Cornell Nanoscale Science and Technology Facility, Marohn's group has successfully fabricated single crystal silicon cantilevers with a force sensitivity of  $S_F \sim 5 \times 10^{-18} \text{ N}/\sqrt{\text{Hz}}$  at a temperature of 4.2 K. The Marohn group has also demonstrated batch fabrication of integrated submicron magnetic tips [52]. This work has given the Marohn group five years' experience in advanced nanofabrication techniques and two years' experience with electron beam lithography.<sup>12</sup> The Marohn team has considerable expertise in MRFM experiments [65, 97], including one of the world's most sensitive measurements of nuclear magnetic resonance [55].

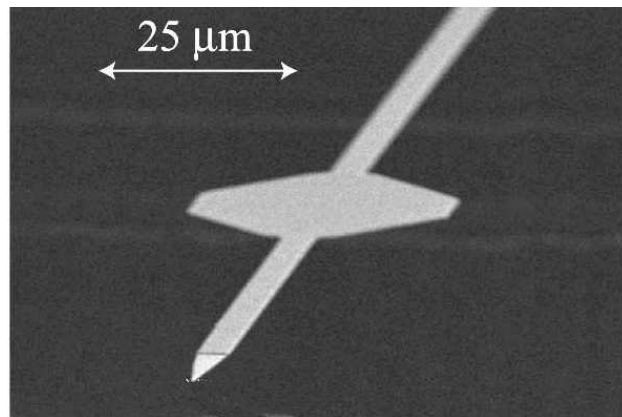


Figure 3 A nanoscale MRFM cantilever fabricated by John Marohn's MRFM Group at Cornell.

### Digital Control and Emulation

The UW MRFM Group has for many years been a world leader in the digital emulation and control of audio-frequency cantilevers [11, 12, 35]. This month (November 2004), the UW MRFM Group passed a milestone with our first PhD thesis demonstrating emulation and control of MRFM cantilevers with MHz frequency [50].

It is standard practice in control engineering to develop emulators and controllers in parallel, using each to debug the other [15]. For our program the main practical advantage is that when the advanced cantilevers are fabricated, the controllers to use them in MRFM experiments will be ready; this tactic improves the overall pace of research and development, and allows MRFM cantilevers to be fabricated with good confidence that will perform as specified.

### End-To-End Quantum Simulation

It is remarkable (and gratifying) that agreement between MRFM theory and experiment has been excellent ever since MRFM began in 1992 [82]. The key ideas of MRFM theory have proven so stable that the advanced Larmor device analyzed in this proposal (as summarized in the far-right-hand column of Table 4) is unchanged from the first design analysis of MRFM ever published [94].

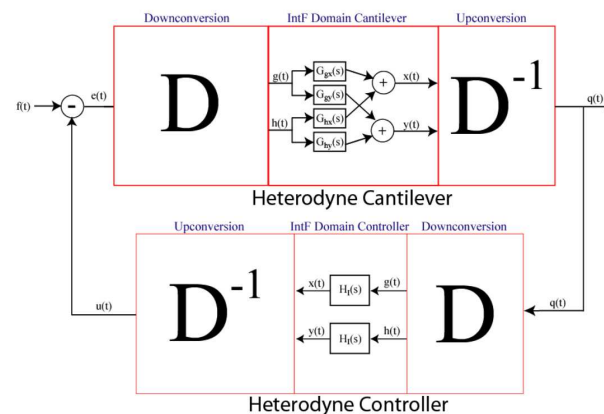


Figure 4 Closed-Loop digital control and emulation

<sup>12</sup>From *The Toyota Way* [61, p. 40]: "Become a learning organization through relentless reflection (*hansei*) and continuous improvement (*kaizen*)."

At left in Figure 5 is a quantum simulation from the pioneering 1992 analysis [94], showing an atomic-resolution 3D scan of an CD4 receptor molecule binding to HIV virus peptide. Such scans are still the ultimate goal of MRFM technology.

We now have a much better understanding of the nature of quantum measurement in MRFM, and the figure at right in Figure 5 shows a very recent end-to-end simulation of the IBM single-electron-spin iOSCAR experiments [81].

These results were presented at the QuIST Workshop in Phoenix on November 19. The agreement between MRFM theory and MRFM experiment remains excellent.

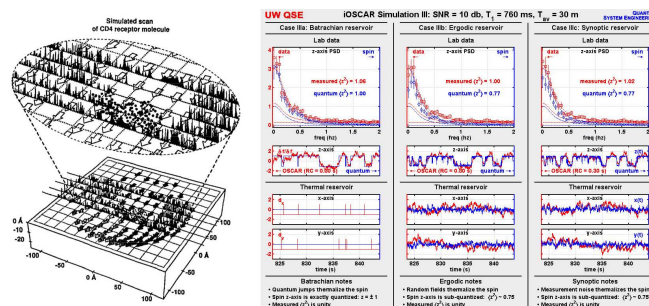


Figure 5 Progress in end-to-end quantum simulation of MRFM, from 1992 (left) [94] to 2004 (right).

### Signal Processing and Imaging Analysis

Under the direction of Al Hero [6, 19, 21, 38–43, 45, 58–60, 77, 85], and with quantum theory from John Sidles, our program aims to develop an integrated image formation and image reconstruction system for bringing MRFM on-line as a future-generation molecular imaging modality. To attain the exquisitely high spatial resolution made possible by recent experiments reported by our collaborators at IBM, a dramatically new approach to imaging needs to be developed that explicitly accounts for non-linear quantum models and measurement noises, and work on such models is well underway [44, 100, 101].

As an example of how our team will work together, we anticipate that strongly nonlinear spin-spin interactions in complex polymer molecules, and also quantum zero-point motions of polymer side chains, will be major challenges for MRFM image reconstruction. We propose to meet these challenges by, first, merging our expertise in signal processing and image reconstruction (Hero) with our expertise in quantum dynamics and measurement theory (Sidles). Then we will implement our quantum imaging models in the environment of our real-time DSP cantilever simulations (Garbini). The anticipated good agreement between these simulations and actual MRFM experiments will motivate and guide our nanoscale cantilever design and fabrication (Marohn). And finally, our whole team will put our theories and our hardware to the test in realistic MRFM imaging trials.<sup>13</sup>

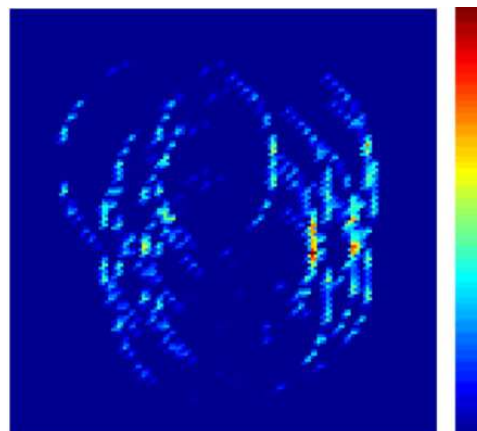


Figure 6 Advanced MRFM imaging analysis from the Hero group.

<sup>13</sup>Alex Warren in *The Toyota Way* [61, p. 237] “If you’ve got a project that is supposed to be implemented in a year . . . Toyota will spend nine to ten months planning, then implement in a small way—such as with a pilot project—and be fully implemented at the end of the year, with virtually no remaining problems.”

**V.3 Quantitative MRFM Design Rules** It is a considerable challenge to optimize the performance of MRFM devices. The design rules must be “as simple as possible, but not simpler.” Our design rules and metrics have the following features:

- (1) The design rules are obtained by optimizing quantitative performance metrics.
- (2) The performance metrics are based on signal-to-noise (SNR) and channel capacity.
- (3) These metrics are solidly grounded in information theory and in quantum physics.
- (4) The quantum limits to MRFM performance are thereby established.
- (5) The goal of single-nuclear-spin detection lies well within the quantum limits.

We will find that the MRFM devices designed by these rules make good sense from the viewpoint of engineering and program management. Our design analysis will confirm the correctness of the original design principles of single-nuclear-spin MRFM [92, 94], provide rigorous foundations for these principles in quantum measurement and information theory, and provide a clear roadmap for continuing MRFM’s track record of exponential progress.

In deriving and explaining our design rules (which for convenience are summarized in Tables 2–4) we will touch upon most of the main challenges in single-spin detection by MRFM.<sup>14</sup> These challenges will largely determine the detailed strategy of our program.<sup>15</sup>

***Programmatic Implications of MRFM Design Rules*** Our design rules will establish that MRFM technology has intrinsically large quantum capacity margin, *i.e.*, that single-spin detection can be achieved by MRFM devices having noise levels that are substantially in excess of the limits imposed by quantum mechanics (see the discussion following (2d)).

This quantum capacity margin substantially mitigates the overall technical risk of single-nuclear-spin MRFM development.

**Remark:** In view of the potentially transformational consequences of the resource mobilization provided by molecular imaging technologies, the discovery that MRFM technology has large quantum capacity margin substantially strengthens the strategic motivations for its development.

**V.4 MRFM Design Parameters** We begin by describing the hardware, sample, and noise parameters of MRFM technology.

***Hardware Parameters*** Consulting Table 2, we see that four parameters describe the MRFM hardware: the motional mass  $m$ , frequency  $\omega_0$ , and quality  $Q$  of the cantilever, and the magnetic gradient  $g$  of the tip. We will find that it is advantageous to make the mass

<sup>14</sup>Fujio Cho in *The Toyota Way* [61, p.149] “Mr. Ōno was passionate about [the Toyota production system]. He said you must clean up everything so that you can see problems. He would complain if he could not look and see and tell if there is a problem.”

<sup>15</sup>In recent weeks we have discussed MRFM development with many different audiences:

ARL : TRANSFORMATIONAL BIOSENSOR TECHNOLOGIES	10/18/04
IDA : BIODEFENSE QUESTIONS AND ANSWERS	10/19/04
DARPA : QUANTUM RADAR FOR MOLECULES	10/20/04
Cornell : BOOTS-ON-THE-GROUND SYSTEM ENGINEERING	10/22/04
QuIST Workshop : THE DYNAMICAL POINT OF VIEW IN QUANTUM SPIN SYSTEMS	11/18/04
UW Bioengineering : ASPECTS OF QUANTUM MICROSCOPY	01/11/05

The tough questions these audiences asked greatly helped us to improve and clarify our development strategy.

and frequency small and the quality and gradient large; the precise scaling of the net device capacity will emerge from our performance analysis.

**Sample Parameters** Two parameters describe the sample spins: the single-spin magnetic moment  $\mu$  and the number of sample spins detected  $n_s$ . Since Program Topic 6 focuses on single-spin detection [73], at the end of our calculations we will always assume  $n_s = 1$ .<sup>16</sup> The choice of magnetic moment  $\mu$  will mainly involve the choice between carbon nuclei (<sup>13</sup>C) and protons (hydrogen nuclei). These are the two most attractive targets for single-nuclear-spin imaging in polymers (we regard biological molecules as a specialized class of polymers); such polymers will be the main focus of our program research.

**Noise Parameters** Two final parameters describe the noise: the process noise spectral density  $S_f$  and the measurement noise spectral density  $S_q$ . We define process noise to be the sum of all random forces  $f(t)$  (thermal or otherwise) acting on the cantilever, and the measurement noise  $q(t)$  to be the sum of all noise processes in the cantilever position sensor.

**Derived Device Parameters** Now we will define (and give motives for defining) several auxiliary device parameters; they are defined wholly in terms of the fundamental device parameters (see Table 2 for details). We first define cantilever spring constant  $k$ , the force  $f_{\text{sig}}$  deriving from a single-spin, and a net process noise  $S_f^{\text{net}}$ ; this latter quantity will appear in the expression for the SNR of single-spin detection using the iOSCAR technique [81].<sup>17</sup>

**Natural Noise Scales** With regard to noise levels, from a physical point of view we always want to know whether a given noise level is “large or small”, and therefore a key question in MRFM design is “large or small noise relative to what reference levels?”

Anticipating a future design rule (derived later on in (2a–2d) starting on p. 17), Table 2 defines a reference process noise  $S_f^{\text{QCL}}$  and measurement noise  $S_q^{\text{QCL}}$  to be the noise levels that yield the maximum MRFM channel capacity.

For the present, we note that  $S_q^{\text{QCL}}$  and  $S_f^{\text{QCL}}$  saturate the *standard quantum limit* (SQL), namely, the fundamental inequality of quantum measurement theory

$$S_f S_q \geq \hbar^2/4. \quad \text{the standard quantum limit (SQL)} \quad (1)$$

The least possible value for  $S_f^{\text{QCL}}$  is therefore (trivially)  $S_q^{\text{QCL}} = \hbar^2/(4S_f^{\text{QCL}})$ . Now the question is reduced to, what noise level  $S_f^{\text{QCL}}$  would make a single-spin MRFM experiment work as well as possible? We will show in (2a–2d) that the expression for  $S_f^{\text{QCL}}$  given in Table 2 *is* this optimal noise level.

With  $S_f^{\text{QCL}}$  and  $S_q^{\text{QCL}}$  in hand, we can conveniently express the experimental noise levels  $S_f$  and  $S_q$  in terms of the dimensionless ratios  $\mathcal{R}_f$ ,  $\mathcal{R}_q$ ,  $\mathcal{R}^{\text{net}}$ , and  $\mathcal{R}^{\text{bal}}$  as defined in Table 2.

Physically speaking,  $\mathcal{R}^{\text{net}}$  may be thought of as the “net” noise level. The standard quantum limit (1) implies  $\mathcal{R}^{\text{net}} \geq 1$ , and from a design point of view it will always be advantageous to operate with  $\mathcal{R}^{\text{net}}$  as near as possible to unity.  $\mathcal{R}^{\text{bal}}$  is the “balance” noise level: its optimal value is unity, with larger values associated with excess measurement noise, and smaller values associated with excess process noise.

<sup>16</sup>However, in deriving our design rules and performance metrics we will retain arbitrary values of  $n_s$ , because future MRFM technologies will likely involve multiplexed modulation of several spins within the resonant slice, and we want to be able to predict the performance gains resulting from such multiplexing.

<sup>17</sup>In all the MRFM designs that we will consider  $S_f^{\text{net}} \simeq S_f$  to an excellent approximation.

Table 2: Summary of device parameters in the MRFM design space.

Hardware parameters			units
mass	$m$	cantilever motional mass	kg
frequency	$\omega_0$	cantilever resonant frequency	rad/s
quality	$Q$	cantilever quality	unity
magnetic gradient	$g$	magnetic gradient of tip	T/m
Sample parameters			
spin moment	$\mu$	magnetic moment of target spin	J/T
sample size	$n_s$	number of spins modulated	unity
Noise parameters			
measurement noise <sup>a</sup>	$S_q$	measurement noise spectral density	$\text{m}^2 \cdot \text{s}$
process noise	$S_f$	force noise spectral density	$\text{N}^2 \cdot \text{s}$
Derived device parameters			
cantilever spring constant		$k = m\omega_0^2$	
single-spin force signal <sup>b</sup>		$f_{\text{sig}} = \mu g$	
net equivalent process noise <sup>c</sup>		$S_f^{\text{net}} = S_f + k^2 S_q / Q^2$	
measurement noise at the } quantum capacity limit }		$S_q^{\text{QCL}} = \hbar^2 / (4S_f^{\text{QCL}})$	
process noise at the } quantum capacity limit }		$S_f^{\text{QCL}} = 0.2610 \times f_{\text{sig}} [n_s m \omega_0 \hbar]^{1/2}$	
excess measurement noise <sup>d</sup>		$\mathcal{R}_q = S_q / S_q^{\text{QCL}}$	
excess process noise		$\mathcal{R}_f = S_f^{\text{net}} / S_f^{\text{QCL}}$	
net excess noise		$\mathcal{R}^{\text{net}} = \mathcal{R}_q \times \mathcal{R}_f$	
noise balance		$\mathcal{R}^{\text{bal}} = \mathcal{R}_q / \mathcal{R}_f$	
<sup>a</sup> Our spectral densities are two-sided, such that $E[q^2] = \int_{-\infty}^{\infty} d\omega / (2\pi) S_q(\omega)$ .			
<sup>b</sup> A vector spin moment $\boldsymbol{\mu}$ in a inhomogeneous field $\mathbf{B}$ exerts a vector force $\mathbf{f}$ having components $f_j = \sum_i \mu_i \nabla_i B_j$ . Given $\hat{\mathbf{n}}$ the axis of cantilever tip motion, it is conventional to define a scalar effective gradient $g$ such that $\mathbf{f} \cdot \hat{\mathbf{n}} \equiv f_{\text{sig}} = \mu g$ is exact.			
<sup>c</sup> The $1/Q^2$ term is negligible for typical devices; it is included for completeness.			
<sup>d</sup> Values for $\mathcal{R}_f$ , $\mathcal{R}_q$ , $\mathcal{R}^{\text{net}}$ , and $\mathcal{R}^{\text{bal}}$ are often stated in decibels, <i>e.g.</i> , $10 \log_{10} \mathcal{R}_f$ (dB).			

**V.5 Summary of MRFM Performance Metrics** Now we have defined all the parameters we will need to compute the performance metrics that will guide our research and development program. The following performance metrics apply not only to our proposed devices, but to *any* MRFM device.<sup>18</sup> To anticipate, in Sections V.6–7 and in Figure 7 we use these metrics to provide a strategic view of the global MRFM design space. For convenience, the metrics are summarized in Table 3.

**The iOSCAR Signal-to-Noise Metric** The most important of the signal-to-noise metrics is the SNR of an iOSCAR-type experiment [81] (see top of Table 3).

The great advantage of iOSCAR-type experiments is their near-perfect immunity to a broad class of technical noise mechanisms. This immunity arises because the iOSCAR modulation technique “toggles” the spin state, such that the signal’s fundamental frequency occurs at *half* the modulation frequency. Since the dominant technical noise mechanisms do not have this “togglng” characteristic,<sup>19</sup> near-perfect suppression of undesired modulation feed-through is obtained. In the first single-spin MRFM experiments [81] signal averaging times of many hours proved feasible, such that large signal-to-noise ratios were obtained. The iOSCAR-type spin toggling technique is very general, and we plan to use it all our MRFM experiments.

However, the iOSCAR SNR is not a suitable metric for design purposes, because it depends crucially on a parameter extrinsic to the MRFM device, namely, the time constant  $\tau$  of the phase-locked-loop used to observe the iOSCAR signal.

External parameters are undesirable in design metrics because they obstruct objective comparisons. For example, the iOSCAR time constant can be varied arbitrarily from experiment to experiment; this variation obstructs us from adopting the iOSCAR SNR as an objective metric. If we seek to eliminate  $\tau$  by maximizing the SNR, we find arbitrarily large SNR for  $\tau \rightarrow \infty$ . This would imply an experiment of infinite duration, which is unphysical.

A commonly-quoted metric that eliminates  $\tau$  is the root-mean-square force noise  $f_{\min}$  within a one-hertz bandwidth. This metric too is included in Tables 3–4. However,  $f_{\min}$  has two undesirable features: first, the one-hertz bandwidth is an arbitrary convention, and second, because quantum mechanics places no limit on  $f_{\min}$ , it is not possible to estimate a device’s quantum capacity margin from  $f_{\min}$ .

**Intrinsic Signal-to-Noise Metrics** To create better performance metrics, we consider that in imaging the rate at which information is acquired is more important than the SNR. In single-spin imaging, we want to acquire—as rapidly as possible—just one bit of information: is a spin present, or not? This motivates us to focus on *channel capacity metrics*. Physically speaking, channel capacity metrics [34, 64] regard each sample spin as a transmitter, and the channel capacity is the number of bits-per-second that the spin can transmit.

As a digression (but one that respects MRFM tradition), Table 3 defines a force-based quasi-capacity metric  $\mathcal{C}^f$  that is proportional to the ratio<sup>20</sup>  $f_{\text{sig}}^2/f_{\min}^2$ . Physically speaking,

<sup>18</sup>Taichi Ōno in *The Toyota Way* [61, p.140] “Standard work sheets and the information contained in them are important elements of the Toyota production system. For a production person to be able to write a standard work sheet that other workers can understand, he or she must be convinced of its importance.”

<sup>19</sup>Commonly observed examples of non-toggling modulation feed-through include thermomechanical cantilever excitation and magnetomechanical coupling between the applied radio fields and the cantilever.

<sup>20</sup>The definition of  $\mathcal{C}^f$  includes a normalizing factor of  $n_s/\ln(2)$  that provides a seamless connection to the

Table 3: Summary of MRFM performance metrics.

**MRFM performance metrics based on signal-to-noise (SNR)**

$$\left. \begin{array}{l} \text{iOSCAR SNR}^a \text{ for phase-} \\ \text{lock-loop time constant } \tau \end{array} \right\} \text{SNR} = \frac{32f_{\text{sig}}^2\tau}{\pi^2 [S_f^{\text{net}} + (2m\omega_0/\tau)^2 S_q]}$$

$$\text{rms force noise in 1 Hz} \quad f_{\text{min}} = (2S_f^{\text{net}}/(1 \text{ second}))^{1/2}$$

$$\left. \begin{array}{l} \text{heuristic MRFM capacity,} \\ \text{as estimated from } f_{\text{min}} \end{array} \right\} \mathcal{C}^f = \frac{n_s}{\ln 2} \frac{f_{\text{sig}}^2}{2S_f^{\text{net}}} = \frac{n_s}{\ln 2} \frac{f_{\text{sig}}^2}{f_{\text{min}}^2} \times \frac{1 \text{ bit}}{\text{second}}$$

**MRFM performance metrics based on channel capacity**

$$\left. \begin{array}{l} \text{net Shannon-Hartley} \\ \text{MRFM capacity} \end{array} \right\} \mathcal{C}^{\text{S-H}} = \mathcal{C}^{\text{QCL}} \times \mathcal{D}^{\text{loss}}$$

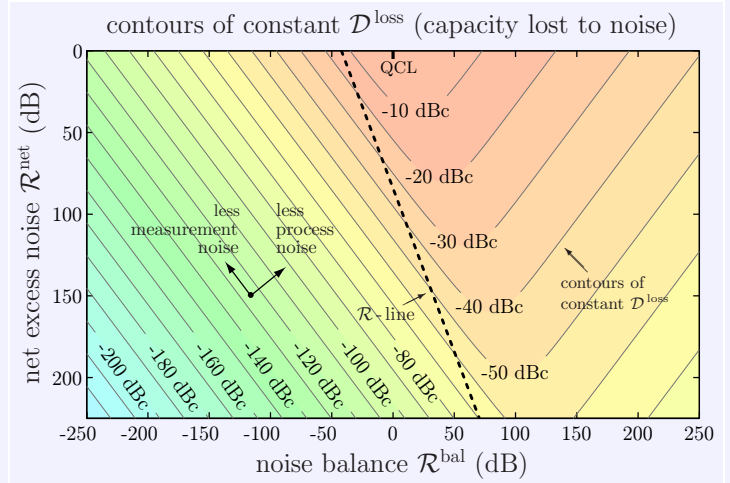
$$\text{quantum capacity limit (QCL)} \quad \mathcal{C}^{\text{QCL}} = 0.4758 \times f_{\text{sig}} [n_s/(m\omega_0\hbar)]^{1/2}$$

$$\left. \begin{array}{l} \text{loss}^b \text{ to excess noise (i.e., } \mathcal{R}^{\text{net}} > 1) \\ \text{and noise imbalance (i.e., } \mathcal{R}^{\text{bal}} \neq 1) \end{array} \right\} \mathcal{D}^{\text{loss}} = \frac{1.6413}{(\mathcal{R}^{\text{net}}\mathcal{R}^{\text{bal}})^{1/6}} - \frac{0.5038}{(\mathcal{R}^{\text{bal}})^{1/2}} \times \arctan \left[ 3.2579 \times \frac{(\mathcal{R}^{\text{bal}})^{1/3}}{(\mathcal{R}^{\text{net}})^{1/6}} \right]$$

$$\left. \begin{array}{l} \text{approximate capacity, valid for all} \\ \text{devices to the left of the } \mathcal{R}\text{-line}^c \end{array} \right\} \mathcal{C}^{\text{S-H}} \simeq \mathcal{C}^f$$

**Graphical analysis of  $\mathcal{D}^{\text{loss}}$  (the MRFM capacity lost to noise)**

- dBc units are  $10 \log_{10} \mathcal{C}$ , where  $\mathcal{C}$  is channel capacity in bits-per-second.
- Since  $\mathcal{D}^{\text{loss}}$  is a universal function, any MRFM device occupies a well-defined point on this chart.<sup>d</sup>
- Devices to the left of the  $\mathcal{R}$ -line<sup>c</sup> are process-noise-limited, and satisfy the simple design rule  $\mathcal{C}^{\text{S-H}} \simeq \mathcal{C}^f$ .
- Maximal channel capacity is always located to the right of the  $\mathcal{R}$ -line.<sup>c</sup>
- MRFM designs with a capacity excess of 30 dBc can tolerate excess noise  $\mathcal{R}^{\text{net}}$  as large as 115 dB.



<sup>a</sup>This is the instantaneous output SNR of an iOSCAR phase-lock-loop configured to have a 12 dB-per-octave roll-off with time constant  $\tau$ . Spin-lock is assumed to be sustained for a durations  $t^{\text{lock}} \gg \tau$ .

<sup>b</sup>To minimize round-off error, whenever the numerical argument of the  $\arctan[\dots]$  is  $\lesssim 0.05$ , use instead the second-order series expansion  $\mathcal{D}^{\text{loss}} \simeq 5.8070 \times (\mathcal{R}^{\text{bal}}/\mathcal{R}^{\text{net}})^{1/2} [1 - 6.3684 \times (\mathcal{R}^{\text{bal}})^{2/3}/(\mathcal{R}^{\text{net}})^{1/3}]$ .

<sup>c</sup>The  $\mathcal{R}$ -line bounds the region  $\mathcal{R}^{\text{bal}} \leq 6.3 \times 10^{-5} \sqrt{\mathcal{R}^{\text{net}}}$ , within which  $\mathcal{C}^{\text{S-H}} \simeq \mathcal{C}^f$  to (+0%, -1%).

<sup>d</sup>PDF and EPS versions are at [http://courses.washington.edu/goodall/MRFM\\_sources/QSE](http://courses.washington.edu/goodall/MRFM_sources/QSE).

$\mathcal{C}^f$  seems to be the rate (in bits-per-second) at which an MRFM device can acquire information from sample spins. We will show that this assertion is justified in a broad (but not global) region of MRFM design space. However,  $\mathcal{C}^f$  shares an unphysical feature with other SNR-based measures: quantum mechanics sets no upper bound on  $\mathcal{C}^f$ , and so the quantum capacity margin cannot be determined from  $\mathcal{C}^f$ . Thus  $\mathcal{C}^f$  is an unsatisfactory metric because it is not globally valid in MRFM design space.

**Channel Capacity Metrics** We will now specify a capacity-based performance metric that: (1) is intrinsic and convention-independent, (2) is globally valid in MRFM design space, and (3) realistically and accurately quantifies MRFM's quantum channel capacity. We will also establish that it links seamlessly to the traditional SNR-based metrics given above.

Our starting point is the Shannon-Hartley Theorem [34], which in the context of MRFM asserts that the maximum feasible channel capacity  $\mathcal{C}^{\text{S-H}}$  is given by

$$\mathcal{C}^{\text{S-H}} = \max_{S_f^{\text{signal}}(\omega)} \int_0^\infty \frac{d\omega}{2\pi} \log_2 \left[ 1 + S_f^{\text{signal}}(\omega)/S_f^{\text{noise}}(\omega) \right]. \quad (2a)$$

Here  $S_f^{\text{noise}}(\omega)$  is the total noise spectral density (*i.e.*, process noise + measurement noise, expressed as a net equivalent noise). For MRFM devices near resonance this total noise is

$$S_f^{\text{noise}}(\omega_0 + \delta\omega) \simeq S_f^{\text{net}} + (2m\omega_0\delta\omega)^2 S_q. \quad (2b)$$

The signal power spectral density  $S_f^{\text{signal}}(\omega)$  of the modulated spin signal  $f_{\text{sig}}(t)$  has a functional form that is chosen to maximize  $\mathcal{C}^{\text{S-H}}$ , subject to the net power constraint

$$2 \int_0^\infty \frac{d\omega}{2\pi} S_f^{\text{signal}}(\omega) = n_s f_{\text{sig}}^2, \quad (2c)$$

where  $n_s$  is the number of spins modulated. It is a straightforward exercise in the calculus of variations<sup>21</sup> to establish that (2a–c) imply the following MRFM channel capacity:

$$\begin{aligned} \mathcal{C}^{\text{S-H}} = & \quad \mathcal{C}^{\text{QCL}}(f_{\text{sig}}, m, \omega_0) && \text{the quantum capacity limit (QCL)} \\ & \times \mathcal{D}^{\text{loss}}(\mathcal{R}^{\text{net}}, \mathcal{R}^{\text{bal}}) && \text{the capacity lost to noise.} \end{aligned} \quad (2d)$$

Expressions for  $\mathcal{C}^{\text{QCL}}$  and  $\mathcal{D}^{\text{loss}}$  are given in Table 3. Provided that process and measurement noise satisfy the standard quantum limit (1), it can be shown that  $\mathcal{D}^{\text{loss}} \leq 1$ . We see that  $\mathcal{C}^{\text{QCL}}$  indeed deserves its name of *quantum capacity limit* (QCL): it is the maximal bit rate permitted by quantum mechanical noise in the measurement process.

**The Channel Capacity of iOSCAR Experiments** The channel capacity of a single-spin iOSCAR experiment can be readily and accurately estimated via the excellent approximation  $\mathcal{C}^{\text{S-H}} \simeq 1/\tau^{\text{iOSCAR}}$ , where  $\tau^{\text{iOSCAR}}$  is the phase-lock-loop time constant required to achieve an iOSCAR SNR of 6.5 dB (note: the needed expression for the iOSCAR SNR appears in the top line of Table 3). This approximation is accurate within (+1.7, -1.3) dBc, and provides a seamless link between channel capacity theory and iOSCAR experiments.<sup>22</sup>

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Shannon-Hartley Theorem.

<sup>21</sup>The variational calculation makes use of Gallager's Water-Filling Theorem [34].

<sup>22</sup>See, *e.g.*, the values for  $\mathcal{C}^{\text{S-H}}$  and  $\tau^{\text{iOSCAR}}$  in Table 4, which satisfy  $\mathcal{C}^{\text{S-H}} \simeq 1/\tau^{\text{iOSCAR}}$ .

**Graphical Tools for Performance Analysis** It greatly simplifies MRFM design that  $\mathcal{C}^{\text{S-H}}$  factorizes into a capacity  $\mathcal{C}^{\text{QCL}}$  that depends only on the hardware parameters, times a dimensionless loss factor  $\mathcal{D}^{\text{loss}}$  that depends only on the noise parameters; this allow us to set separate MRFM performance goals for hardware and noise. The design parameters of Table 2 were carefully chosen to achieve this factorization, which illustrates a general principle of system engineering: *design rules themselves require careful design*. In this section we borrow graphical techniques that are widely used in aircraft design<sup>23</sup> and apply similar techniques to the design of MRFM devices.

Table 3 provides a contour-plot of the function  $\mathcal{D}^{\text{loss}}(\mathcal{R}^{\text{net}}, \mathcal{R}^{\text{bal}})$ . This contour-plot is universal in the sense that it applies to all MRFM devices.

Examining the contour-plot, we see that approaching the quantum capacity limit (QCL) requires  $\mathcal{R}^{\text{net}} = \mathcal{R}^{\text{bal}} = 1$ , *i.e.*, the noise must both saturate the standard quantum limit ( $\mathcal{R}^{\text{net}} = 1$ ) and be balanced between process noise and measurement noise ( $\mathcal{R}^{\text{bal}} = 1$ ). When process noise dominates measurement noise ( $\mathcal{R}^{\text{bal}} \ll 1$ ), the Shannon-Hartley capacity  $\mathcal{C}^{\text{S-H}}$  is asymptotically equal to empirical capacity  $\mathcal{C}^f$  given previously; the  $\mathcal{R}$ -line of the contour-plot demarks the region of agreement (see footnote *c* of Table 3 for details).

**MRFM’s Large Quantum Capacity Margin** Strikingly evident on the contour-plot of Table 3 is MRFM’s large quantum capacity margin: a capacity loss of 30 dB is consonant with a net excess noise as large as 115 dB.

This extraordinarily large “headroom” is unique among emerging quantum technologies, and is a defining aspect of MRFM’s emerging strategic roles.<sup>24</sup> For the engineering community, large quantum capacity margin means that further MRFM development work need not await fundamental breakthroughs in quantum physics and mathematics (although breakthroughs are welcome, of course),<sup>25</sup> and can begin to focus on many equally challenging but non-fundamental issues that relate to technical noise and MRFM system design.

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<sup>23</sup>The chief inspiration for our capacity metrics and graphical tools is John Boyd’s pioneering aircraft design synthesis [23, 46]. In particular, the plots of Table 3 and Figure 7 are conceptually similar to Boyd’s plots of specific excess power (SEP), which are widely used in designing fighter aircraft [3, 7, 79]. Broadly speaking, less overall MRFM noise  $\mathcal{R}^{\text{net}}$  corresponds to greater aircraft altitude, the quantum limit  $\mathcal{R}^{\text{net}} = 1$  corresponds to an altitude ceiling, and greater or lesser values for the MRFM noise balance  $\mathcal{R}^{\text{bal}} = 1$  correspond to greater or lesser aircraft velocity (note that too much “velocity” and too little “velocity” are bad for both technologies). Finally, just as aircraft designs are summarized by SEP as a function of altitude and speed, MRFM designs are summarized by  $\mathcal{C}^{\text{S-H}}$  as a function of  $\mathcal{R}^{\text{net}}$  and  $\mathcal{R}^{\text{bal}}$ .

Thus, both SEP metrics and  $\mathcal{C}^{\text{S-H}}$  metrics summarize multiple design considerations. In Boyd’s language, the lessons-learned for MRFM are these: (1) MRFM’s large quantum capacity margin creates plenty of “maneuvering energy” in design space (2) Strategies for MRFM development should seek to make optimal use of this maneuvering energy.

<sup>24</sup>From *The Toyota Way* [61, p. 137]: “This time [is] an opportunity to study alternatives and have them ready to go when the styling design is frozen. It is called the *kentou* (study drawing phase) and the focus in this period is generating hundreds of study drawings, called *kentouzu*.”

<sup>25</sup>The boundary between engineering and science is diffuse, and historically this boundary has provided fertile territory for young investigators. For example, the Green function methods developed during WWII by Julian Schwinger [68] for engineering purposes relating to radar waveguides played a pivotal role in his post-war contributions to quantum field theory. As John Bardeen advised young scientists [47]: “[Most advances] are made in response to a need, so that it is necessary to have some sort of practical goal in mind while the basic research is being done; otherwise it may be of little value.” Understanding the quantum aspects of MRFM imaging will, we foresee, provide precisely this sort of fertile investigative territory for developing the next generation of young scientists and engineers.

Table 4: Survey of MRFM device parameters and performance metrics.

Hardware parameters <sup>a</sup>	metric	units	IBM/UW 1992	UW 1998	Cornell 2004	IBM 2004	QSE acoustic	QSE Larmor	UW RSI 1992
mass	$m$	pg	3.9e4	6.4e3	2.0e3	92	560	4.4 <sup>b</sup>	6e-3 <sup>c</sup>
frequency	$\omega_0/2\pi$	hz	8.0e3	7.7e3	850	5.5e3	1.5e3	1.0e6	7.1e6
quality	$Q$	1	2000	2.2e4	4.4e4	3.0e4	1.0e5	1.0e5	2.0e6
gradient	$g$	mT/nm	1.0e-5	0.25	0.028	0.20	10	42	42
temperature	$T$	K	300	77	4	1	0.1	0.1	0.03
<b>Spin parameters</b>									
spin magnetic moment <sup>d</sup>	$\mu$	10 <sup>-26</sup> J/T	1.4	1.4	1.4	1.4	1.4	1.4	0.35
<b>Noise parameters</b>									
measurement noise	$(S_q)^{1/2}$	pm/ $\sqrt{\text{hz}}$	1	1	1	10	1	1	1
process (force) noise <sup>e</sup>	$(S_f)^{1/2}$	zN/ $\sqrt{\text{hz}}$	4.1e6	2.4e5	7.8e3	6.7e3	540	2.2e3	16
<b>Derived device parameters</b>									
spring constant	$k$	mN/m	100	15	0.06	0.11	0.05	185	12
single-spin force signal	$f_{\text{sig}}$	zN	1.4e-4	3.5	0.39	2.8	141	590	150
QCL measurement noise	$(S_q^{\text{QCL}})^{1/2}$	pm/ $\sqrt{\text{hz}}$	3.2	3.2e-2	0.22	0.11	1.4e-2	4.5e-3	2.8e-2
QCL process noise	$(S_f^{\text{QCL}})^{1/2}$	zN/ $\sqrt{\text{hz}}$	0.032	3.24	0.47	0.92	7.42	23	3.6
excess measurement noise	$\mathcal{R}_q$	dB	-10	30	13	39	37	47	31
excess process noise	$\mathcal{R}_f$	dB	162	98	84	77	37	40	13
net excess noise	$\mathcal{R}^{\text{net}}$	dB	152	128	97	116	74	87	44
noise balance	$\mathcal{R}^{\text{bal}}$	dB	-172	-68	-72	-38	0	7	17
<b>Signal-to-noise (SNR) metrics</b>									
iOSCAR observation time <sup>f</sup>	$\tau^{\text{iOSCAR}}$	sec	5.7e20	3.3e9	2.8e8	3.9e6	10.2	9.9	0.02
rms force noise in one hz	$f_{\text{min}}$	zN	4.1e6	2.4e5	7.8e3	6.7e3	540	2.2e3	16
<b>Channel capacity metrics</b>									
quantum capacity limit	$\mathcal{C}^{\text{QCL}}$	dBc <sup>g</sup>	-53	-5	-6	4	20	20	26
capacity lost to noise	$\mathcal{D}^{\text{loss}}$	dBc	-152	-90	-77	-69	-30	-30	-11
net capacity ( $\mathcal{C}^{\text{QCL}} + \mathcal{D}^{\text{loss}}$ )	$\mathcal{C}^{\text{S-H}}$	dBc	-205	-95	-83	-66	-10	-10	15

<sup>a</sup>The first four columns, labeled ‘IBM/UW/1992’ [82], ‘UW/1998’ [9], ‘Cornell/2004’ [36], and ‘IBM/2004’ [81], illustrate past achievement in MRFM. The next two columns, ‘QSE/acoustic’ and ‘QSE/Larmor’, are the designs of this program. The final column, ‘UW RSI/(1992)’ [94] is the most complete Larmor design analysis in the literature.

<sup>b</sup>A silicon Larmor cantilever of length 25  $\mu\text{m}$ , width 600 nm, and thickness 500 nm, at 100 mK.

<sup>c</sup>A 1992 SiO<sub>2</sub> Larmor design, of length 2.8  $\mu\text{m}$ , and width = thickness = 57 nm, at 30 mK.

<sup>d</sup>All single-spin signals are proton moments, except the final column, which is <sup>13</sup>C.

<sup>e</sup>For columns 1–4, this is observed noise [9, 36, 81, 82], not the noise inferred from temperature.

<sup>f</sup>Here  $\tau^{\text{iOSCAR}}$  is defined to be the phase-lock-loop time constant required to observe a single nuclear spin with an SNR of 6.5 dB. As noted following (2d) on pp. 17,  $\mathcal{C}^{\text{S-H}} \simeq 1/\tau^{\text{iOSCAR}}$ .

<sup>g</sup>A dBc is defined to be  $10 \log_{10} \mathcal{C}$ , where  $\mathcal{C}$  is a channel capacity in bits-per-second.

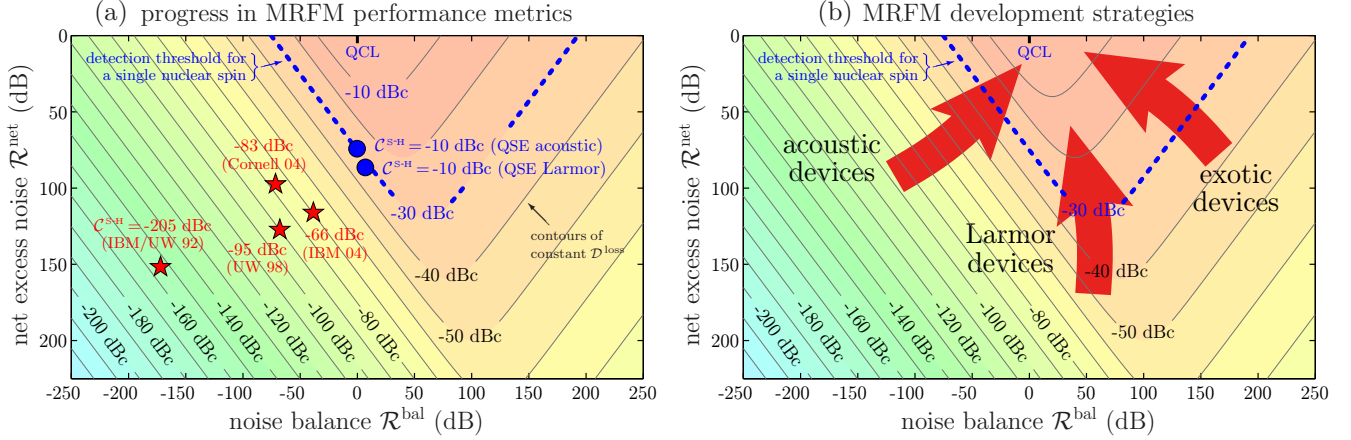


Figure 7: Overview of MRFM designs and development strategies.

- (a) The MRFM designs of Table 4 (stars and circles), labeled by their single-nuclear-spin channel capacity  $\mathcal{C}^{\text{S-H}}$ , and plotted at their noise coordinate  $(\mathcal{R}^{\text{bal}}, \mathcal{R}^{\text{net}})$ . See footnote 23 (p. 18) for a discussion of similarities to John Boyd’s aircraft design methods.
- (b) Three strategies for MRFM development and deployment. See Sections V.7–8.

**V.6 MRFM System Design in a Nutshell** We propose to improve the single-nuclear-spin capacity metric from its present value of -55 dB (achieved in the IBM experiment [81]) to -10 dB, which is the capacity value established by that same IBM experiment as adequate for the goal of single spin detection. We will pursue two designs:

- (1) *acoustic cantilevers*, operating at audio frequencies, for which spin-lock is achieved by external application of a radio-frequency field [81], and
- (2) *Larmor cantilevers*, operating at MHz frequencies, for which spin-lock is achieved (at least partly) via radio-frequency fields generated by cantilever vibrations [94].

**Hardware Performance Goals** With reference to the quantum capacity  $\mathcal{C}^{\text{QCL}}$  values given in Table 4, our design goal is to improve  $\mathcal{C}^{\text{QCL}}$  by 16 dBc, from the present value of 4 dBc to the design goal of 20 dBc.

The rationale for pursuing two MRFM hardware designs is apparent in Table 4, namely, next-generation acoustic and Larmor designs offer similar hardware capacity  $\mathcal{C}^{\text{QCL}} \sim 20$  dBc. Therefore, during the base period we propose to fabricate both types, deferring until the option period a downselection to a preferred design. The downselection will be based primarily on the noise performance established during the base-period imaging trials.

**Noise Performance Goals** With reference to the values for capacity lost to noise  $\mathcal{D}^{\text{loss}}$  given in Table 4, our design goal is to improve  $\mathcal{D}^{\text{loss}}$  by 39 dBc, from the present value of -69 dBc to the design goal of -30 dBc. The design path is via lower temperatures and moderately higher cantilever quality. Most of the required  $\mathcal{D}^{\text{loss}}$  improvement comes indirectly, via the “retuning” of the reference noise levels  $S_q^{\text{QCL}}$  and  $S_f^{\text{QCL}}$  in consequence of the above hardware changes. In particular, these devices will be the first to operate near the optimal noise tuning  $\mathcal{R}^{\text{bal}} \simeq (\mathcal{R}^{\text{net}})^{1/2}$  that is so strikingly evident in the  $\mathcal{D}^{\text{loss}}$  contour-plot.

**V.7 Relation to Existing Knowledge** We envision MRFM development as a three-way competition between two conservative strategies (acoustic *versus* Larmor cantilevers) and a third class of exotic device designs. The exotic designs have in common high measurement noise and low process noise; hence they approach the quantum capacity limit from the right-hand-side ( $\mathcal{R}^{\text{bal}} \gg 1$ ) of Figure 7b.<sup>26</sup>

The result is a three-way “horse race” in MRFM development. To the extent that comprehensive 3D imaging with single-nuclear-spin sensitivity proves feasible, this race is being run for planetary-scale stakes in defense, science, medicine, and economics. MRFM technology’s large quantum capacity margin, exponential progress, and clear development path all strongly suggest that this race *will* have an eventual winner.

In consequence, MRFM is becoming recognized as one of the most exciting and dynamic of all science and engineering disciplines. In our view, it is reasonable to anticipate that the three-way MRFM technology race will emerge as one of the 21st Century’s Grand Challenges, uniting and applying a broad spectrum of research in applied physics, chemistry, nanoscale science, quantum science and technology, and system engineering.

***The Nanofabrication and Sensing Challenge*** The key nanoscale elements of MRFM technology have been demonstrated separately: cantilevers, tips, and sensors. The grand MRFM challenge is to realize these elements in combination.

***The Materials Science Challenge*** Noise-related MRFM parameters are at present determined semi-empirically: cantilever  $Q$ , tip-sample relaxation mechanisms, and spin decoherence. The grand MRFM challenge is to understand the physics of this noise, and mitigate it, such that the quantum capacity limit can be approached.

***The Quantum Science and Information Challenge*** MRFM is now entering a regime in which the dynamical effects of quantum measurement compete with the traditional dynamical effects of spin-spin interactions and spin-lattice interactions. The grand MRFM challenge is to modulate and optimally extract this nonlinearly encoded information.<sup>27</sup>

**V.8 Relation to Defense Missions** In the development of radar—a technology of sophistication and transformational consequence similar to MRFM—Beyerchen [4] has noted that “the key to [turning] a discovery or invention into successful [military] innovation lies in whether laymen can envision its possibilities.” We will now attempt to envision how an

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<sup>26</sup>Examples of exotic strategies include ultralow-mass cantilevers fabricated of, *e.g.*, nanotubes; levitated magnetic spheres; and non-mechanical approaches, *e.g.* [95]. We do not propose to develop exotic devices, but neither do we regard these approaches as infeasible *prima facie*.

<sup>27</sup>As engineers, our QSE group is severely challenged by the (approximately) three thousand new articles on quantum measurement theory that appear each year [49]. This extraordinary level of activity amounts to a continual explosion of creative discovery. For us as quantum system engineers, the struggle to assimilate this ever-expanding literature is a source of *muda* (non-value-added effort), *muri* (labor without insight), and *mura* (irregularity of action, unnaturalness) [61, p. 114].

A central goal of our QSE group’s quantum science and information research is to mitigate this *muda*, *muri*, *mura*—insofar as feasible—by distilling those aspects that are well-validated into design rules that are optimized for professional quantum system engineering.

This task is made easier by the emerging recognition [76, 80, 99] that quantum measurement theory contains equivalence classes [2, 8, 18, 25, 57, 98] that allow synoptic distillation of the literature. This distillation is a major focus of our present research. We call this goal “quantum system engineering without *muda*, *muri*, *mura*” and it is a central organizing principle of our “pursuit of engineering perfection.”

MRFM imaging technology might perform in a deployed military setting.

Deployed MRFM imaging units surely will be compact, because an MRFM scanner fits comfortably in the palm of a hand. We anticipate that power needs for cryogenic cooling will be modest; a few kilowatts at most. The exponential rate of MRFM progress suggests (and quantum mechanics allows) that each individual unit will have a 3D molecular imaging capacity of hundreds of coordinates per second, with this capability becoming available in the five-year to ten-year time scale.

Figure 8 depicts a bioresponse battery that might be deployed in the time-frame 2010–2015. We attempted to envision how the role of specialist class USMC MOS 5711 “nuclear biological and chemical (NBC) defense specialist” would be transformed by access to this unit. We determined that MRFM-based molecular imaging would give platoon-scale units more biocapability than the entire Human Genome Project. The transformational impact of such a “radar for molecules” capability is obvious.<sup>28</sup>

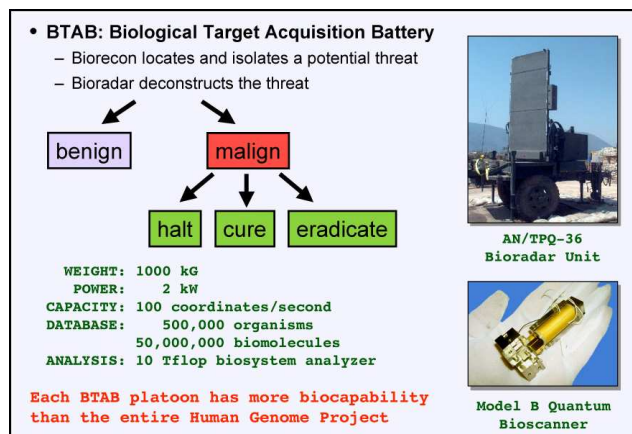


Figure 8 An MRFM bioresponse battery.

**V.9 Educational Approach** Nine graduate-level engineering degrees, each with a thesis topic specifically focussed on MRFM, have come out of the UW MRFM Group [14, 17, 20, 50, 51, 53, 63, 75, 83]. We believe this number is more than any other MRFM research program.

We anticipate that the proposed program, supplemented with in-place NIH and NSF funding by Sidles and Marohn, will support 8–10 graduate students in each year. Our curriculum is hands-on and fast-paced, and we seek to develop high morale among our young engineers [103, p. 231]. An important objective of this white paper—possibly its most important objective—is to provide principled foundations for this morale-building.

## VI Project Schedule and Milestones

**VI.1 Base Period** During the three-year base period we will design, implement and evaluate the hardware components of a single-nucleon experiment: low-mass/high-gradient cantilevers, and a low noise cryogenic imaging environment.

Because our present design studies show that single-nucleon detection might be achieved by either acoustic or Larmor frequency cantilevers, we will begin by evaluating both.

<sup>28</sup>Our thinking in this section is strongly influenced by an official DoD history: *The United States Army in World War II* [103]. The first volume is entitled *Chief of Staff: Prewar Plans and Preparations*, and the DoD had an objective in writing it [103, p. IX] that this white paper also attempts to serve:

“The second objective [of this series] is to help enlarge the thoughtful civilian’s concept of national security by describing the basic problems of war and the methods of meeting these problems.”

As thoughtful civilians, the authors of this white paper are impressed by the parallels between WWII radar development and MRFM development. Just as radar was envisioned as an urgently-needed means for military and civil defense against aircraft threats [103, p. 38], MRFM can be envisioned as an urgently-needed means for military and civil defense against chemical and biological terrorist threats.

Also like radar—but to an even greater extent—MRFM technology promises to provide new foundations for the national and global economic prosperity upon which modern military strategy relies [71].

Tasks	Who			Year 1				Year 2				Year 3				Year 4				Year 5			
	UW	CU	UM	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
<b>Design &amp; Apparatus</b>																							
scanner modifications	●			■	■	■	■																
cantilever/tip fabrication																							
acoustic		●		■	■	■	■	■	■	■	■					■	■	■	■				
Larmor		●		■	■	■	■									■	■	■	■	■	■	■	■
<b>select:</b> Larmor or acoustic																●							
interferometer development	●			■	■	■	■	■	■	■	■												
technical noise mitigation	●																						
300mK refrigerator design	●			■	■	■	■																
refrigerator install/test	●							■	■	■	■												
<b>select:</b> refrigerator or cryostat																				●			
<b>Spin Physics Experiments</b>																							
technical noise studies	●	●		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
acoustic cyclic saturation	●			■	■	■	■																
acoustic iOSCAR-type exp.	●							■	■	■	■	■	■	■	■								
Larmor spin-locking exp.	●	●						■	■	■	■	■	■	■	■								
single-nucleon detection	●	●	●													■	■	■	■	■	■	■	■
<b>single-nucleon:</b> go/no go																				●			
<b>Theory &amp; Analysis</b>																							
single-nucleon analysis	●	●	●	■	■	■	■																
multi-nucleon analysis	●	●	●					■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
technical noise analysis	●		●					■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
<b>Signal Processing</b>																							
signal processing	●		●	■	■	■	■	■	■	■	■												
DSP & control	●		●	■	■	■	■																
image reconstruction	●		●																	■	■	■	■

Table 5: The proposed program timeline.

**Design and Apparatus** The UW’s closed-loop 3D MRFM scanner will be modified to accept both acoustic and Larmor frequency cantilevers for single-nuclear-spin imaging. Focused cantilever interferometry capable of sensing small-target cantilevers will be implemented (Garbini).

In addition, working with a commercial vendor, we will adapt our experiment to operate in a 300 mK  $^3\text{He}$  pulse tube refrigerator. Although vibrations will be challenging, our present analysis indicates that, with careful design, sufficient isolation can be achieved. Installation will occur during Y2Q3.

Simultaneously, high-gradient acoustic cantilevers ( $f_0 = 1.2$  kHz,  $k = 60$   $\mu\text{N}/\text{m}$ ,  $g = 10$  g/Å) and then Larmor cantilevers ( $f_0 = 1$  MHz,  $k = 6000$   $\mu\text{N}/\text{m}$ ,  $g = 20$  g/Å) will be fabricated (Marohn). By Y2Q1, we will be ready for nuclear spin experiments at  $T = 10$  K in our existing cryostat.

**Spin Physics Experiments** Initial studies will center on mitigating technical noise (feedthrough and close-approach sample noise) to levels consistent with single-nucleon detection for both acoustic and Larmor cantilevers. We will begin with acoustic iOSCAR-type experiments, and proceed to Larmor spin-locking experiments as the cantilevers become available. As part of these tests we will conduct 3D imaging trials at 100, 10, and 1 nm resolutions. We will begin our imaging studies with samples consisting of polymer films on silica: as thin a monolayer or as thick as a bulk sample. Depending on the results we will extend the range of samples to encompass both conducting and semiconducting poly-

mers and biological molecules. The goals of the experiments during the base period will be to resolve two issues: (1) Is single-nucleon MRFM detection/imaging feasible with either acoustic or Larmor frequency cantilevers? (2) Which of the two techniques is best suited for single-nucleon tests during the two-year option?

**Theory and Analysis** Profs. Hero and Sidles will lead the effort to create an end-to-end model of the single-nuclear-spin imaging process, including potentially thorny dynamics issues like dipole-dipole spin interactions and zero-point motion of polymer length segments, extending through the quantum-classical interface to the interferometric imaging process, continuing through wholly classical control of the cantilever, and terminating in signal detection and image deconvolution .

**Signal Processing** The spin physics models developed by Hero and Sidles will be implemented on the existing UW DSP system. This will allow us to emulate MRFM cantilevers in advance of their fabrication. Our goal is to reliably predict and emulate in real time a broad class of MRFM experiments. This capability will substantially speed the development effort.

**VI.2 Option Period** During the two-year option period, with the hardware in place, we will finalize the experiment design and concentrate on technical noise issues.

**Noise Reduction** Our primary goal will be to reduce technical noise to within 30 dBc of the quantum capacity limit. Although that noise level will allow detection of single nuclei, further improvement may be necessary for practical imaging.

**Single-Nucleon Detection** We will continue to improve the experiment as necessary to demonstrate single-nucleon detection in a practical imaging environment. Likely alterations might include optimization of cantilever/tip design, improved electro/optics to reduce measurement noise, and increased scanner resolution.

**VI.3 Project Milestones** Table 6 gives project milestones and dates.<sup>29</sup>

Table 6: Project Milestones

Milestones for the Three Year Base		Date
Milestone 1:	Finalize integrated development platform	Y2Q1
Milestone 2:	Larmor and acoustic cantilever/tip fabrication	Y3Q4
Milestone 3:	Imaging at 100, 10, and 1 nm resolution	Y1Q4, Y2Q4, Y3Q4
Milestone 4:	Validated spin physics and noise budgets	Y3Q4
Milestone 5:	Larmor versus acoustic downselection	Y3Q4
Milestones for the Two Year Option		
Milestone 6:	Approach the quantum capacity limit within 30 dB	Y4Q4
Milestone 7:	Demonstrate single nuclear spin detection	Y4Q5

<sup>29</sup>With respect to the syllabus that began this white paper (Section II), the lessons learned are:

SCIENCE : Our program’s objective is difficult, yet time-honored and important.  
 BUSINESS : To succeed, we must relentlessly pursue perfection, eliminating *muda, muri, mura*.  
 DEFENSE : Our objective is technology that provides transformational access to new resources that will help defend against “hunger, poverty, desperation, and chaos . . . so as to permit the emergence of political and social conditions in which free institutions can exist” [66].

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