COMPUTING

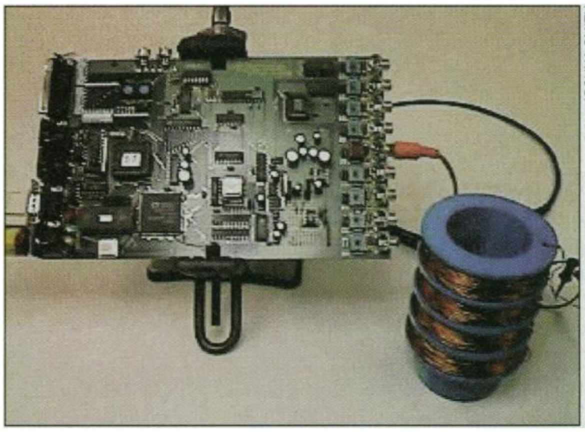
Putting a Quantum Computer To Work in a Cup of Coffee

Like most things that sound too good to be true, quantum computing comes with some exasperating fine print. The famous quantum weirdness of the microscopic world allows a computer to follow many different paths at once, collapsing calculations that would take billions of years on mundane supercomputers into a few seconds—at least in theory. But the experimental reality has been less encouraging. After heroic experimental efforts, physicists have managed to create individual quantum logic gates—in essence, single transistors based on quantum principles—that can handle all of two bits of data (*Science*, 7 July 1995, p. 28). The situation has been summed up succinctly by Massachusetts Institute of Technology (MIT) computer scientist Seth Lloyd in his not-quite-immortal phrase: "A two-bit microprocessor is a two-bit microprocessor."

Now, the world of quantum computing may be undergoing a paradigm shift. Two groups of researchers have independently come up with a way to turn mundane liquids into quantum computers of 10 to 20 quantum bits. The key is nuclear magnetic resonance (NMR), a technique that is already a mainstay of medical imaging and chemical analysis. Described in this issue of *Science* by MIT's Neil Gershenfeld and Isaac Chuang of the University of California, Santa Barbara (p. 350), and in an upcoming *Proceedings of the National Academy of Sciences* paper by Tim Havel and Amr Fahmy of Harvard Medical School together with David Cory of MIT, the strategy in effect paves the way for the first quantum circuits. While these circuits are still not enough to do interesting calculations—10 bits, says Lloyd, "is totally great for factoring the number 15"—they should open up new test-beds for quantum computation.

Cory, Fahmy, and Havel have actually built quantum circuits using a standard NMR spectrometer, while Gershenfeld and Chuang are gearing up experiments and hope to demonstrate quantum circuits and maybe even a simple computation by next summer. The researchers note that fundamental obstacles may prevent the scheme from ever producing a practical computer. But "from the point of view of verifying the basic ideas and doing interesting physics," says Lloyd, a pioneer theorist in quantum computing, "it's fantastic."

The new technique, like all quantum computing, relies on the superposition principle of quantum mechanics, which maintains that until it's measured or observed, any quantum system—the spin of a nucleus or the energy of an electron, for example—can exist in a superposition of all its possible states at once. While a classical bit in today's computers must be either a 0 or a 1, a single quantum-mechanical bit—a qubit—simultaneously contains a 0 component and a 1 component, and n quantum-mechanical bits can simultaneously represent 2^n numbers. Because the qubits can evolve along many paths at once, they should be able to perform calculations on all 2^n bits at once—a feat known as quantum parallelism. "There isn't anything known outside of quantum mechanics where that happens," says Havel.



JOSHUA SMITH

Fresh-brewed. A prototype tabletop NMR quantum computer, showing the circuitry and the radio-frequency coil.

The fine print in this case is that any interaction between a qubit and the macroscopic world sparks a process known as decoherence, collapsing the quantum superposition to a classical state. "A quantum computer has to do something apparently impossible," says Gershenfeld. "Its bits have to be isolated completely from the environment so they don't decohere, but they need to be accessible so you can load them, move them around, and interact with them."

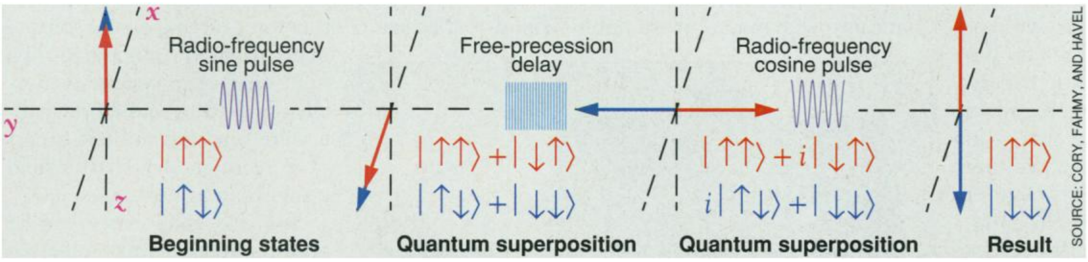
Of a half-dozen attempts so far to reconcile these two demands and build a quantum logic gate, two have succeeded. A collaboration at the National Institute of Standards and Technology (NIST), led by David Wineland and Chris Monroe, has created a single quantum gate out of an electromagnetically trapped beryllium ion, whose spin—up or down—represents 0, 1, or a superposition of the two. At Caltech, physicists Jeff Kimble and Quentin Turchette have made a gate from photons that can be polarized vertically or horizontally. But both of these experiments, as Chuang points out, required extraordinarily complex technology and exotic conditions to isolate and manipulate the qubits.

Spinmeisters. From the early days of quantum computing, NMR was an obvious candidate to do the job without the heroics. The gist of NMR is that the nuclei of atoms behave like little bar magnets, with north and south poles. "When you take a sample and put it into a magnet," says Havel, "the spins gradually begin to align with the field." Because of other forces acting on the spins—in particular, the random jostling from heat—the system eventually comes to an equilibrium with a mere one-in-a-million excess of spins aligned with the field rather than against it.

But this small excess can be manipulated using electromagnetic pulses at radio frequencies. Send in a pulse at the right frequency—it varies with the type of element and the environment of the nuclei—and some of the nuclear spins will flip around into the opposite orientation. When the pulse ends, these spins are left precessing—wobbling—like an assembly of tiny gyroscopes. In the process, they generate an electromagnetic signal that can be detected. "You can watch that happen and collect a spectrum," says Havel, which is how NMR spectroscopists learn details of a sample's composition and molecular structure.

As Lloyd and David DiVincenzo of IBM both pointed out, NMR systems provide two crucial advantages for quantum computing. First, the up-or-down spin of the atomic nuclei is, as quantum systems go, unusually long-lived. In other quantum systems, decoherence sets in within milliseconds, if not pico- or femtoseconds. "Here you have one and the same quantum phase lasting up to thousands of seconds," says Gershenfeld. "The reason is that the spins in the nuclei are beautifully protected from the rest of the world. Electrons around them screen them from the environment, and their rapid tumbling averages out the external interactions."

What's more, the various spins present in a molecule are "coupled" together, so that the frequency at which one spin might flip can depend on the state of neighboring spins. An isolated carbon nucleus might shift at one frequency, for instance; a carbon nucleus near a hydrogen nucleus might shift at the same frequency if the hydrogen's spin points



New spin on logic. In an NMR version of a controlled-NOT gate (also known as an XOR gate), a pair of radio-frequency pulses flips a nuclear spin (blue) or leaves it unchanged (red) depending on the state of a second spin. Each spin stores one bit of information, with up spins representing a 0 and down spins, 1.

down but at a different one if the hydrogen's spin points up. By choosing which precise frequency to broadcast to the carbon nucleus, says Lloyd, "what you get is a kind of logic. You flip the carbon, for instance, if, and only if, the hydrogen is up." That's the essence of what's called a controlled-NOT gate, a basic component of computers.

The quantum advantage comes in because radio pulses of the right frequencies can also put the spins they address into a particular superposition of states, in which they are both up and down simultaneously. Any spins that are coupled to that superposition will also move into a superposition of both up and down states. "Now you have a weird quantum state," explains Lloyd, "carbon up plus hydrogen up, and carbon down plus hydrogen down, a totally weird quantum state without a classical analog." This quantum gate can now operate on all its possible values simultaneously.

The actual quantum circuit is then constructed not in space, by hooking up one quantum gate to another, but in time. "The bits stay in one place," says Gershenfeld, "and you bring in pulses" that trigger the logical operations of each gate individually, then construct a new gate from the same set of spins, by changing which spins are flipped conditional to which other spins. "We have all these different types of interactions that we can apply selectively by using pulses," says Gershenfeld. "You can view it as switching on and off the interactions between spins."

Lost in the crowd? But again, there's the fine print. Quantum computing requires that the bits being worked with start off in what quantum mechanicians call a "pure" quantum state, in which all the spins point in a known direction—a situation very different from the one in NMR, where at most a small fraction of the spins can be aligned. "At room temperature and even at very, very low temperature, spins are largely randomized, pointing in all directions," says Lloyd. Nor is there any way to home in on, manipulate, and read out the spins of individual nuclei within that disorderly crowd. "The input and output problems seemed insurmountable," says Lloyd. Chuang calls it "the ultimate garbage-in, garbage-out problem."

That two groups came up with solutions virtually simultaneously suggests it was an idea whose time had come. At Harvard Medical School, Havel, a computational biophysicist, and Fahmy, a computer scientist, had moved into quantum computing when they learned that the Defense Advanced Research Projects Agency was looking to fund work in the field. When they came up with what Havel calls "concrete theoretical ideas to be tested," they went looking for "the best NMR-methods person" they could find, and were put in touch with Cory at MIT.

Down the road at MIT's Media Lab, Gershenfeld had been working with Sensormatic, the company that makes anti-shoplifting tags. The tags contain a metallic glass whose nuclei resonate, giving off a tiny radio signal, when a tag passes through an oscillating magnetic field on the way out of a store. "It got me thinking," says Gershenfeld. "Since I'm talking to spins to do a simple job in magnetoelastic tags, could I go further and do information processing with the spins?" He had an eager collaborator in Chuang, who had been working on quantum computation since his undergraduate days in the late 1980s.

Last spring, both groups identified the key to introducing and extracting something more than quantum garbage from an NMR sample. As Chuang puts it, "The eventual solution was so natural and simple, it was almost as if it existed already and was trying to express itself. A very strange feeling."

What the researchers realized is that they could use that small statistical excess, the one part in a million, of the spins that are preferentially pointing in the direction of the magnetic field. Precisely because most of the molecules in the sample are tumbling and jiggling randomly, they can be ignored: Their quantum variables average to zero. "It turns out having a well-defined statistical excess of a single quantum state is enough to do quantum computing," says Havel. "You don't need to have every molecule doing exactly the same thing. If you read any elementary freshman text on NMR spectroscopy, you'll see that they often talk about the spins in a liquid as if there were only one molecule present, even though the system is physically much more complicated."

To turn this insight into quantum logic, the NMR spectroscopists need nothing more than a sample filled with simple molecules that contain a handful of spins—the caffeine in coffee is a favorite pedagogical example. "You put a cup of coffee between the plates of a big magnet," says Lloyd. "Now you perform this trick: You beam in the frequency that different types of spin listen to, conditional on the states of other spins. You can look at spins three, four, five, and six on the molecule, for instance, conditional on the states of spins one and two. You can guarantee if spins one and two are both up, then the other spins are in a pure state." The result is a simple quantum circuit, ready to be programmed.

The read-out problem is solved by listening to all the molecules in the coffee at once, rather than trying to listen to one spin at a time as with other quantum-computing schemes. "It's not so hard to measure spin number four on some molecule if you have nearly Avogadro's number of that molecule," says DiVincenzo. And the quantum computationalists can take their time listening to the ensemble, says Gershenfeld, because the act of listening—the quantum-mechanical measurement, in a sense—doesn't force the quantum states to collapse to classical states as it would if just one molecule or nucleus was being measured. "You can do something very strange" with the quantum bits, he says. "You can continuously measure them, continuously read them out."

As Havel, Cory, and Fahmy reported last November at a Boston workshop on physics and computation, they have already turned common liquids into logic gates and done simple operations. So far, they have worked with up to four bits, he says, and should be able to achieve 10 to 20 easily by using more complex molecules. The catch is that the read-out signal generated by the nuclei in the molecules gets weaker exponentially as the number of spins in the molecule increases. In effect, exponentially more information has to be read from the same number of molecules. "Already at 10 bits," says Lloyd, "your output is down by a factor of 1000; at 20, it's down by a factor of a million; 30 spins, you're down by a billion. Unless you start taking heroic experimental measures, you won't detect the signals."

But it's beyond 30 bits where real computation starts. "Somewhere between 50 and

100 bits is where calculations start to get interesting," says Gershenfeld, who agrees that, without some very clever new development, the best an NMR-based quantum computer will ever do is tickle the lower end of that range. To get even that far, he says, an NMR-based system will have to be cooled to near absolute zero or use new algorithms. Says NIST's Monroe, "This NMR scheme is pretty slick stuff, but in the long run they're going to have to find a particularly special molecule or state that allows them to extend it to large numbers."

Still, what can be done now can be done with easily available and affordable equipment—"off-the-shelf coffee cups, off-the-shelf liquids, off-the-shelf magnets, etc.," says Lloyd—and it will open the way to testing new algorithms proposed for quantum computation and studying the properties of bizarre multiple-spin quantum states that until now have been untouchable. And if researchers can figure out how to extend the technology to larger bit numbers, says Gershenfeld, the future is unlimited. While traditional computer scientists struggle to squeeze more and more devices on a chip (see p. 303), NMR-based quantum-mechanical computing holds the promise of letting nature do all the work. "We're just computing more powerfully by being smarter about what nature allows us to do."

–Gary Taubes

ARCHAEOLOGY

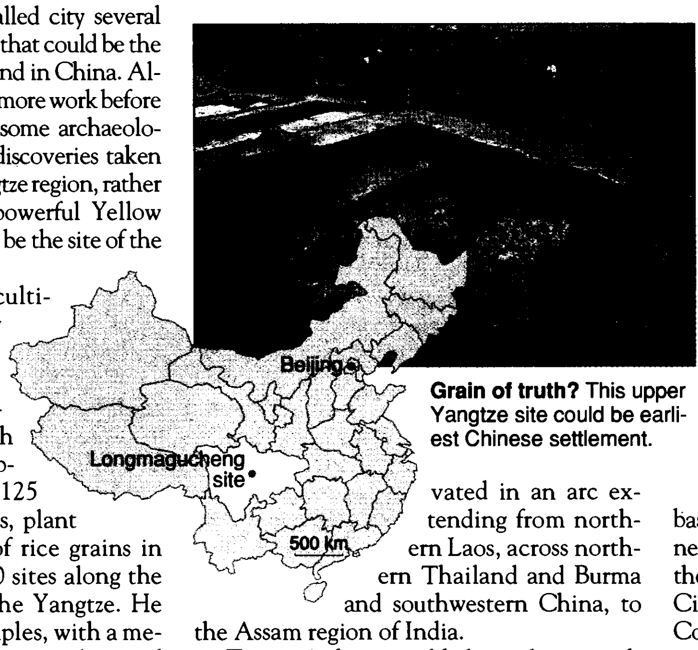
Yangtze Seen as Earliest Rice Site

NARA, JAPAN—The cultivation of rice—a potent symbol of civilization for many Asian nations—may have occurred first along the middle Yangtze River in central China, according to preliminary findings by a team of Japanese and Chinese archaeologists. If confirmed, the findings, described at an international meeting* held here last month, would move back the date—and narrow the location—of the earliest domestication of this important crop.

Evidence for very early rice cultivation in the region may mesh with another find described at the meeting: a walled city several hundred kilometers upstream that could be the oldest such settlement yet found in China. Although both finds need much more work before the claims can be accepted, some archaeologists speculate that the two discoveries taken together suggest that the Yangtze region, rather than the more politically powerful Yellow River area to the north, could be the site of the oldest civilization in China.

This new view of rice cultivation was described by Syuichi Toyama, an environmental archaeologist at Japan's Kogakukan University. Toyama surveyed both published and recent unpublished radiocarbon data on 125 samples of rice grains, husks, plant remains, and impressions of rice grains in pottery from more than 100 sites along the 5400-kilometer length of the Yangtze. He reported that the oldest samples, with a median age of 11,500 years, are clustered along the middle Yangtze in Hubei and Hunan provinces. Samples from sites both upstream and downstream are typically younger, dating from 4000 to 10,000 years ago. That pattern, says Toyama, suggests that rice cultivation originated in the middle Yangtze and spread from there.

The work "is very important, and the fact that the dates are coming from a series of sites is persuasive," says Ofer Bar-Yosef, an archaeologist at Harvard University's Peabody Museum. Bruce Smith, an archaeologist at the Smithsonian Institution in Washington, D.C., who has written on the origins of agriculture, says that evidence has been mounting for the last decade that the Yangtze was probably the site of the earliest rice cultivation. But until very recently, the oldest evidence of Yangtze rice cultivation went back only 8000 years. The new findings are also likely to further refute earlier theories that rice was first cultivated in an arc extending from northern Laos, across northern Thailand and Burma and southwestern China, to the Assam region of India.



Grain of truth? This upper Yangtze site could be earliest Chinese settlement.

Toyama's dates would also make rice cultivation along the Yangtze older than the millet cultivation of northern China, which dates back 7800 years. It could also predate the earliest known agricultural site in west Asia—the domestication of barley 10,000 years ago. Bar-Yosef says that determining where and when rice cultivation began could help to explain the environmental, climatic, and perhaps social conditions that fostered its emergence. "The questions that are left open concerning the agricultural revolution 10,000 years ago in China are: What caused it? What led to this change?" he says.

The second component of the Yangtze findings—claims that early rice cultivation in the region nurtured an ancient, lost civilization—stand on more tenuous evidence. "It needs more work," says Fekri Hassan, an archaeologist at University College, London, who heard the presentations in Nara. A team excavating a site called Longmagucheng, along the upper reaches of the Yangtze about 35 km southwest of Chengdu in Sichuan Province, believes it may have identified the ruins of a fortified town with an earthen wall. Near the center of the enclosed area, which measures 1100 by 600 meters, is a three-tiered earthen platform that the researchers believe served some religious or governmental ceremonial function.

Unpublished radiocarbon dating of soil taken from the walls and the earthen platform place the site at between 4500 and 5000 years ago, says Yoshinori Yasuda, a geographer who heads the Japanese side of the team. Although that is younger than ancient civilizations in the Middle East, it would be older than anything yet found in China. Indications of urban settlements suggest that it was more advanced, and thus probably older, than a civilization believed to have existed along the Yellow River in northern China, says Yasuda.

The dig is being carried out by the Kyoto-based International Research Center for Japanese Studies, Sichuan Union University, and the archaeological department of Chengdu City. It is funded entirely by Japan's Kyocera Corp., a high-tech ceramics-maker, to promote cross-cultural understanding.

While intrigued, other archaeologists want to see more evidence. Harvard's Bar-Yosef says that a city of that size should also show evidence of houses, storage facilities, and refuse pits. "We're just at the very start," says Chaolong Xu, a Chinese archaeologist trained at Kyoto University who is a member of the Longmagucheng team. Xu foresees more than a decade of excavations at this and nearby sites in the valley to determine the region's role in human history.

–Dennis Normile

* International Symposium on Agriculture and Civilizations, Nara, Japan, 13–14 December 1996.