About

Founded in 2004, Nanorex Inc. is a developer of open-source computational modeling tools for the design and analysis of atomically precise nanosystems. The members of the Nanorex team share a common vision - to create compelling, reliable, affordable and easy to use engineering software to support the development of advanced nanotechnologies on the pathway to productive nanosystems.Mission

- Our mission is to support the design and development of advanced nanosystems
- DNA structures can provide frameworks for next-generation nanosystems
- Structural DNA nanotechnology is a point of high leverage for computational tools
- An open-source framework will enable collaborative development of software tools

Nanorex is developing open-source computational tools to support research in structural DNA nanotechnology (SDN). To do this, we are extending our existing application, NanoEngineer-1, to provide a foundation of tools for visualization, modeling, and manipulation of DNA, and to make it a framework that can support and integrate other computational tools developed by the SDN community. This work is part of our broader mission to support the development of advanced nanosystems. We've entered a process of collaborative development that will help the SDN research community integrate its diverse tools for design, modeling, and analysis, making them more useful and more widely available. Working with the rest of the SDN community, we'd like to make this process serve everyone's needs at multiple levels, both as users and as developers. Our mission is to support the design and development of advanced nanosystems

Self-assembled atomically precise nanosystems hold great promise in many areas, both experimental and practical. Among the products will be systems that help researchers build more advanced systems. We expect structural DNA nanotechnology to play a central role in next-generation nanosystems.

Our mission is to support the design and development of advanced nanosystems through computational tools. In all areas of technology, tools for design and modeling help researchers to solidify their ideas into concrete representations and to evaluate and revise them. This speeds the cycle of design, fabrication, and testing at the center of the development process. SDN will be no exception. DNA structures can provide frameworks for next-generation nanosystems

Three lines of research are converging to create a capability for systematic design of complex, atomically precise nanosystems. SDN has a crucial role in this prospective development.

Special structures

The first line of research is the development of a wide range of atomically precise functional components -- organometallic complexes, magic-size quantum dots, nanotubes and fibers, engineered surfaces, and so forth. These have functions ranging from chemical catalysis to electro-optical transduction to structural support. This wide range of functions, however, is offset by a major limitation: each of these functional components is a special structure, either unique or part of a small family, not a member of a designable class of billions of possible structures. This limitation makes it almost impossible to design components that will self-assemble to form complex, atomically precise systems. By themselves, these special structures are simply too constrained to provide the necessary diversity of selectively complementary surfaces.

Engineered proteins

The second line of research is the development of polymers made from a diverse set of monomers that fold to make specific 3D structures. Protein engineering is the advanced technology of this sort, and it has progressed to the point where researchers routinely design novel structures that are more stable than those found in nature. Artificial and natural examples show that proteins can perform a wide range of functions, and can bind proteins, nucleic acids, and an enormous range of other atomically precise structures, both biological and non-biological. Proteins therefore provide a solution to the problem of assembling the special, highly functional structures discussed above. Protein molecules can be effective structures: they have strengths and stiffnesses like those of epoxies, polycarbonates, and other engineering polymers. However, these useful properties are offset by a slow design, fabrication, and testing cycle (several months) and by the small size of individual proteins (a few nanometers). They are attractive as components and linkers, but less attractive as a way to combine components to make large systems.

Structural DNA

The third line is SDN itself, which now can be used to implement a large growing range of structures on a scale of tens to thousands of nanometers. Like proteins, but unlike the special, highly functional structures, DNA is a modular system that can be used to make a set of structures of combinatorial size, with billions of possible design choices for strands just a few nanometers long. Unlike proteins, DNA structures can be made with a fast design, fabrication, and testing cycle (no more than a few days, in some instances), and they can easily be thousands of times larger in volume. They can provide specific binding sites for proteins or DNA-tagged structures, holding hundreds or thousands of components in specific spatial geometries.

These lines of development are complementary, the first providing diverse elements of high functionality, the second providing components that can bind them precisely, and the third providing structures that can organize them in large numbers to form complex patterns. The resulting ability to build modular composite nanosystems opens the door to an as-yet unimaginable range of experimental and practical applications. SDN plays a vital role in this prospect: it is literally what holds it all together. Structural DNA nanotechnology is a point of high leverage for computational tools

DNA structures are a good target for computer-aided design tools. They are regular enough that they can be designed and using relatively abstract representations, yet complex enough that computer support for visualization is essential. With DNA as a medium, designers can arrange and rearrange parts in a systematic way, much as they would in designing conventional macroscopic objects.

Special structures, by contrast, leave little scope for design, and while proteins have enormous scope for design, the process has special difficulties. Where a designer can rearrange DNA strands by following simple rules, relying on the regularities of helical structure and paired bases, a protein designer must use a computational search process to find combinations of side chains that fit together. This makes even the simplest design steps more difficult to plan and implement.

The development of modular composite nanosystems will require computational support for designs that include special structures and proteins, and some support may be possible at an early date. SDN design is the natural starting point, however, and is a rich field in itself. An open-source framework will enable collaborative development of software tools

The growing SDN community has developed many software tools, and will develop many more in the years to come. Nanorex is developing open-source software that provides tools for visualization, modeling, and manipulation of DNA structures, and that provides interfaces for integrating these capabilities with existing and future software tools developed within the SDN community.

Because the core software is open source (NanoEngineer-1 is under GPL), all participants can be confident that it won't become expensive, and that any team that is working to extend it must continue to satisfy the broader community. Nanorex can't take down the project by failing, going bad, or trying to squeeze money out of the software itself -- in the worst case, the work would simply continue under new leadership.

Researchers will want to keep control of the tools they create, both to ensure their quality and to get proper credit when they are used. These tools can be treated as distinct open-source projects, giving researchers full control of the content of software that appears under their names. User interface conventions in NanoEngineer-1 will give clear credit to the creator of a tool when it is used. Rather than absorbing contributions and making them invisible, the project will offer researchers a new distribution channel that can make their work better known, better supported, and more widely used.

Our mission is to support the design and development of advanced nanosystems, and we see SDN is a central part of that development. No single research group or company could possibly provide all the necessary tools, so the choice is whether to have a jumble of incompatible pieces of software, each implementing a limited user interface, or to find a way to bring these tools together to form a more integrated system with powerful capabilities. We think that the general approach described here will enable the second, superior option. The approach itself, of course, is also open to contributions and revision by the community of users and contributors in the SDN research community.