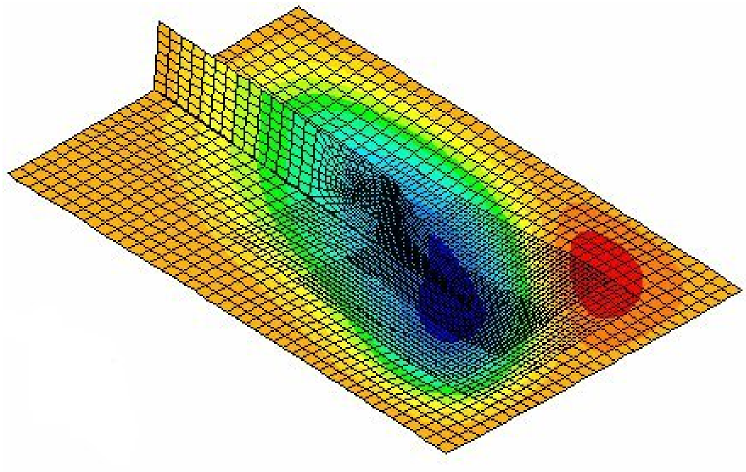

# RESEARCH DIRECTIONS IN COMPUTATIONAL AND COMPOSITE MECHANICS

*A Report of the United States National Committee on Theoretical and Applied Mechanics (USNC/TAM), June 2007*

**This report discusses two aspects of the engineering science of mechanics that have a profound impact on *American Competitiveness*, and addresses issues raised in the National Academy of Sciences report *Rising Above the Gathering Storm*. The United States has played a leading role in the development of computational mechanics and mechanics of composite materials. It is clear that the futures of these two disciplines of mechanics are very bright as they both will have a profound impact on many facets of our life, including advances in biology, medicine, energy conservation and development, and national security. It is also clear that the United States is not the only country working in these advanced fields of engineering science. There are very strong initiatives and commitments to these fields in Europe and Asia. A concentrated effort by the United States is necessary if we are to maintain our competitiveness.**

## Part 1: Computational Mechanics

Over the past 40 years, the landscape of science and engineering has changed dramatically due to the emergence and unparalleled growth of computational hardware and simulation methods. A major driving factor has been the dramatic decrease in the cost of computations, a billion-fold reduction in the last 40 years! At the same time, tremendous improvements in algorithms and computational methods, such as the finite element method, the finite volume method and new solvers, has made it possible to harness this computational power for simulations that have become an indispensable part of engineering and science. Simulations, by replacing tests with computer models, have dramatically reduced the cost of the engineering design process, reduced design cycle times, and have made it possible to address scientific and engineering questions beyond the capabilities of experiments, including, questions related to climate change, the astrophysics of black holes, and many others. The importance of computations in all fields of science and engineering is still growing rapidly, and in fact, it is now widely accepted that computation is becoming the third pillar of science, joining the well-established pillars of theory and experiment.

Computational mechanics has played a pivotal role in simulation-based engineering and design. It has introduced technologies such as finite element methods, computational fluid dynamics and computational fracture mechanics that dramatically increased the capabilities and productivity of industrial practice today. However, many of the most important challenges which offer the greatest potential benefits to society are beyond our current knowledge base. Dramatic leaps are needed in our understanding and capabilities in simulation to address these challenges.

To exemplify this, we will review the status of computational mechanics in three fields:

1. modeling of materials and systems, with an emphasis on multiscale methods
2. predictive medicine
3. simulation of cellular processes

In each case, we will summarize why the field is important, the key challenges and the potential benefits to society. This summary is partially based on references [1] and [2], and especially [3].

**Modeling Materials and Systems:** Simulations of materials and systems are at a strategic crossroad today. Considerable progress has been made in many applications; for example, crashworthiness analysis has saved the auto industry billions of dollars and improved automotive safety, prototype simulation such as droptests and performance simulations have dramatically shortened design cycles. However, the determination of material properties for these simulations often requires tremendous expenditures in time and money. By supplanting much of this testing by multiscale simulations, so that material properties are obtained by simulations at smaller scales, considerable time and money can be saved in design. At the same time, such capabilities will aid in the design of improved materials.

These developments will hinge on improvements in:

1. linking of the scales, especially for unstable material response that characterizes failure, which is known as multiscale methods
2. methods for complex multi-physics simulations

Multiscale methods are generally classified as:

1. hierarchical methods (also called coarse graining and information passing), where fine scale models inform coarser scale models of system parameters, such as material properties
2. concurrent methods, where problems involving different scales are solved concurrently and interactively

Hierarchical methods fall under the broad rubric of homogenization methods. In many applications, the objective is to obtain material properties of a coarse scale model by simulating a fine scale model that contains details such as the microstructure that are beyond the resolution of the coarse scale model. Examples include composite materials, the effects of dislocations, voids and particulates on material response, and biological materials that often have a rich detail of structures at various scales.

The theory of homogenization is well established for linear, periodic, deterministic models. For moderate nonlinearities sound and effective computational procedures have been developed. However, bottlenecks still arise in how to incorporate results from nonlinear fine scale models into coarse-grained models. Generally the amount of computation required for on-the-fly transfer is exorbitant, but pre-computed data bases are often very large and unwieldy. And methods for materials with random non-periodic micro-structure remain an open area of research.

The major barriers in multi-scale methods are how to reduce the complexity of fine scale computations and how to treat instabilities, in particular in the coarse-graining of failure models. Since the determination of the strength of a structure or component is of crucial importance in engineering and science, these barriers needs urgent attention. The difficulties arise because in multiscale simulations of failure, material instabilities at any scale lead to localization of deformation at that scale. Therefore, classical methods of homogenization are no longer applicable and new methods for linking the scales must be developed. A large knowledge base and additional research are required to make multiscale modeling of failure feasible. This is further complicated in that the requirements often involve chemistry and other physical processes.

In concurrent methods, models at various scales are linked within a single computation; the fine scale model is used where the physics requires it, whereas coarser scale models are used where finer scale physics is not considered of interest. These methods are often used with the study of defects or defect propagation. A typical application is the coupled quantum, molecular, continuum model of Khare et al. [4] (Fig.1). Considerable research is still needed in these methods to make them viable. For example, effective interface treatments, in particular for transient thermal problems, are needed between the continuum/molecular/quantum domains. The use of various scales for treating the propagation of defects, for diffusion, and for electromagnetic fields is only in its infancy.

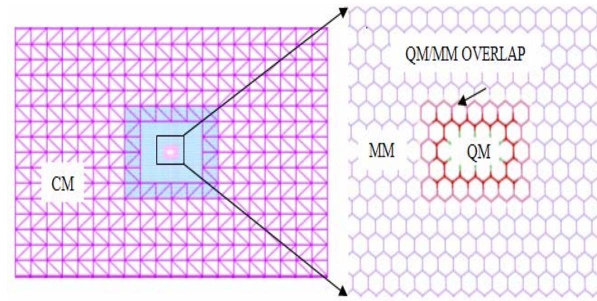


**Figure 1[4]. Coupled QM/MM/CM model of a graphene sheet**

Although quantum computations have long been the domain of theoretical physical chemists and physicists, the involvement of computational mechanicians, both through developments in the quantum methods and their coupling to continuum and molecular methods, is crucial. There is no reason why computational mechanics should be confined to continuum mechanics; the numerical and modeling methods in quantum mechanics could profit immensely from the many techniques developed in computational continuum mechanics.

Direct simulation at small length scales also poses major barriers because of the large time scales that must be considered. Many important phenomena arise from intermittent events. Two examples are the growth of a fatigue crack at the microscale level, and the diffusion of defects in a material or structure. Brute force simulations of such phenomena require excessive amounts of computer time, and it is clear that more effective methods must be developed. Some new methods are being considered, but this is a field in which a major breakthrough is needed.

Some important areas that are perhaps not as central to academic research, but have important industrial applications that were cited in Ref [3] are:

1. rapid model generation
2. dynamically driven data acquisition
3. verification, validation and uncertainty quantification

We will not discuss these here but refer the reader to Ref [3] for more details.

**Predictive Medicine:** The realm of computational mechanics also can provide society great benefits in the fields of biology and medicine. In the realm of medicine we will describe the situation in cardiovascular modeling, one of the most highly developed and important applications of computational mechanics. The success in this area of research is indicative of developments taking place in other areas of biology and medicine.

Cardiovascular disease (CVD) is the leading cause of death of both men and women in the United States and the entire industrialized world. By 2010 it is estimated that it will be the leading cause of death in the developing world as well. In 2002, over 70 million Americans suffered from one or more types of CVD, over 43 million were under the age of 65, approximately 6.4 million were hospitalized, and over 1.4 million died, amounting to 38% of all causes of death [5].

It is not widely known, but CVD is also one of the leading causes of death of children. In 2005 the estimated direct and indirect cost of CVD in the United States alone was approximately $393 billion, making CVD the most costly component of total healthcare spending [5]. Consequently, the understanding and treatment of CVD are subjects of the greatest national and international importance.

The historical and current paradigm in cardiovascular medicine is diagnosis. Physicians use various tests to determine a medical condition and then plan a treatment or intervention based upon experience. There is no attempt to predict an outcome although there may be some statistical data to indicate the success rate of a procedure. Success may be defined in various ways depending on the nature of the treatment. It may be the ability to regain certain bodily functions, or simply survival. However, statistics alone are not reliable predictors of success for individual patients. There is simply too much variability from case to case, especially for diseased patients. The current situation is far from satisfactory.

It is interesting to compare medical practice with engineering. Both are problem-solving disciplines. However, in engineering there is an attempt to accurately predict the performance of a product or procedure. The entire design process is based upon predicted outcomes. Very often a number of criteria must be satisfied simultaneously. Sophisticated computer and analysis technologies are employed.

In comparison with engineering, medical practice is a “build them and bust them” approach. It is inevitable that this will change, primarily because of the emergence of medical imaging technologies, which provides a non-invasive window into human anatomy and physiology. Medical imaging promises to do for the practice of medicine what the telescope did for astronomy and what the microscope did for biology. Medical imaging is already the most important tool for diagnosing CVD and its fidelity and resolution are progressing at a rapid pace. However, the pace has become so rapid that for the newer and higher-resolution technologies, such as the 64-slice CT, there is little or no statistical basis for treatment planning.

It appears inevitable that the practice of medicine in the future will resemble the practice of modern engineering more closely. An example is illustrative. Until fairly recently, research in the simulation of arterial blood flow employed very simple, idealized models and the relevance to medical practice was very limited. Recently, a new era in vascular research was initiated in which realistic, patient-specific models were employed not only to simulate pre-operative, diseased configurations, but also to analyze post-operative outcomes. This has evolved into the concept of "predictive medicine" in which patient-specific simulations are performed to evaluate the efficacy of various possible treatments and to plan and design the optimal intervention based upon computational predictions of outcomes.

Thus far, effort has been focused on modeling major arteries, such as the aorta (see Fig. 2), carotid, iliac, and femoral arteries and the cerebral circulation.

**Figure 2. A model of a patient-specific abdominal aortic aneurysm is obtained from imaging data. A computational model is developed (middle) and calculations of blood flow in the model are performed. Streamlines of the flow at a time instant in the cardiovascular cycle are shown on the right.**

The basic challenges facing the development of predictive medicine is linking medical imaging modalities to engineering simulation technologies, such as geometric modeling, object modeling, automatic and adaptive mesh generation, finite element analysis, computational solid and fluid mechanics, fluid-structure interaction, and interactive, three-dimensional visualization. The integration of these technologies and the presentation of this information to the physician in a useful form are fundamental research questions that need to be answered.

Similar opportunities and challenges have arisen in prosthetics, artificial organs and soft tissue treatments, such a plastic surgery. In all of these areas, predictive medicine can offer great benefits, but a knowledge base and integration of the imaging, and predictive modalities needs to be developed. The shift from the traditional diagnostic paradigm, to a predictive one will revolutionize medical practice by improving outcomes of treatment and reductions in cost, and will be of great benefit to the health and economic well being of the nation and humankind.

**Cellular Processes:** Computational modeling at the cellular scale also offers substantial challenges and benefits. Many of the functions of cells depend on mechanics, one of the keys to their understanding lies in simulation. The study of cellular processes for the past century has been the domain of biology, and a huge body of knowledge has been developed. However, it has been difficult to harness this knowledge because general models have not been available. Useful computational simulation techniques for cellular process will require the synthesis of mechanics, chemistry and other disciplines.

Living cells are made of many sub-cellular components of which two key types are polymerizing and depolymerizing filaments (e.g. actin, microtubules, intermediate filaments), and motor proteins (e.g. myosins, kinesins, dyneins). These components undergo active processes that convert chemical energy into the mechanical mode. For example, actin and tubulin polymerization and depolymerization produce mechanical forces using the free energy of monomer binding and/or nucleotide hydrolysis. Actin and tubulin are also tracks for walking motors, which, powered by the chemical energy of nucleotide hydrolysis, perform specific mechanical tasks such as cargo transport, mitosis, and muscle contraction (Fig. 3).

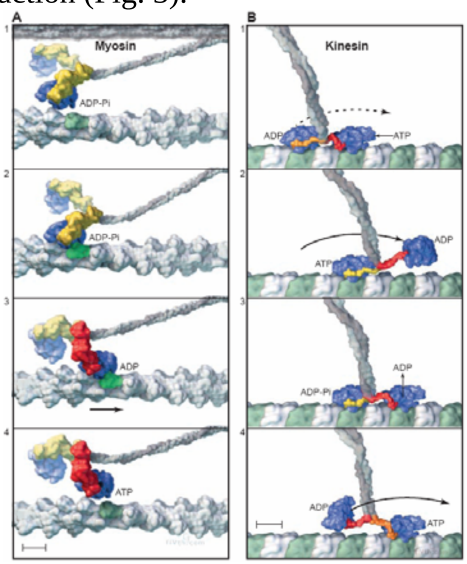


**Figure 3.[6] Configuration changes in walking myosin (left) and kinesin (right).**

The above active components, together with their specific interactions with each other and with the suspending fluid, and the thermal motion result in dynamic self-organized structures that form the cytoskeleton (Fig. 4). Typically, these self-organized structures are driven by chemical energy utilized in the active processes and dissipated in the fluid.

As a result of these microstructural dynamics the cell as a whole has a very complex behavior. It is an active entity that responds to both chemical and mechanical stimuli. Understanding the response of the cell to such stimuli defines the area of cell mechanics. The relationship between mechanics and cell function is a key indicator to differentiate healthy cells from diseased cells, e.g., it is known that the mechanical response of cancer and malaria cells is quite different from regular cells [8, 9]. Behavior of sub-cellular components is also indicative of diseases, e.g., in cancer cells it is thought that mitotic kinesins show enhanced activity [6]. On the other hand, loss of motor function is also linked to neurological, sensory or genetic disorders [6].

The primary challenge is to develop a computational model to interpret the experimental data, to aid in the understanding of the interplay between active bio-chemical processes and the mechanics of the cell as a whole and its components in vivo, and to allow prediction of processes relevant to disease, such as metastases in cancer. Among

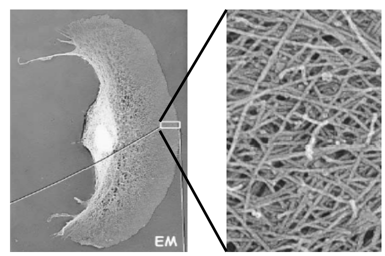


**Figure 4.[7] Left: An electron micrograph of a motile keratocyte. Right: A close-up view of a self-organized actin filament network.**

the computational problems of interest are:

1. modeling of the chemo-mechanical transduction in sub-cellular components such as motor proteins (Fig. 3)
2. modeling cell behavior of dynamic reorganization of the cytoskeleton that is triggered by biochemical processes (Fig. 4).

These and other problems span several decades in spatial and temporal scales, thus they require multiscale methods [10]. Moreover, the mechanical models need to be fully coupled with models of the bio-chemical processes. The field is still in its infancy but stands to benefit significantly from the multiscale computational approaches discussed earlier. Computational models will help elucidate cell function, and thus can have a critical impact on understanding the progress of diseases, their diagnosis and treatment.

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## Part 2: Mechanics of Composite Materials

A composite material can be simply defined as a material consisting of more than one constituent. The distinction as a composite clearly depends upon the scale under consideration. For example, on one level concrete is a homogeneous material; however at a more refined scale, concrete consists of several constituents, including various sizes of aggregates, sand and cement. The human body may be the most exotic example of a composite material consisting of a wide variety of constituents depending upon the scale of interest. Composites appear, or can be made, in a wide variety of forms, including fibrous and particulate configurations.

Composites materials are being used in a wide variety of applications, including civil and military structures, all types of transportation vehicles, aerospace applications, sports equipment, prosthetic devices for replacement of human body parts, and energy generation and conservation devices. Some of these applications will be discussed in this article. The advantages of composites include, but are not limited to, high stiffness and strength, dimensional stability, and near infinite fatigue life.

**Space Applications:** On October 4, 2004, SpaceShipOne (Fig. 5), a fibrous composite spacecraft manufactured by Scaled Composites, rocketed into space, becoming the first manned spacecraft to enter space twice within the span of 14 days. This event was approximately six thousand years after composite materials were first used by Egyptians to make laminated writing materials from the papyrus plant (Ref [11]).

The fact that it took over six thousand years to make these advancements demonstrates the difficulty in developing the underlying science that enables engineers to design and fabricate a light-weight, high-performance structure that is capable of withstanding the rigors of spaceflight, including the temperature extremes of re-entry through the earth's atmosphere. SpaceShipOne is actually ferried up to 50,000 ft. on another all-composite aircraft, White Knight, before being released and rocketed into space.


**Figure 5[12]. SpaceShipOne in flight**

The success of SpaceShipOne is dependent upon the fact that it and its ferry, White Knight, are both composite structures. The composite structures are lighter, stiffer and stronger than metallic structures. In addition, they can be designed to exhibit low or zero coefficients of thermal expansion, exhibit exceptional fatigue life and are less susceptible to corrosive environments.

The innovative design of the composite structure makes it possible to develop a flight pattern such that the spaceship is exposed to lower temperature extremes during re-entry than, say, the NASA Shuttle. In space, the wings of SpaceShipOne fold up providing a shuttle-cock or "feather" (Fig. 6) effect during reentry. This creates extremely high drag during reentry that reduces the temperature exposure of the structure.

An aspect of mechanics discussed in Part 1 of this report is the fact that these planes/spacecraft were designed and *flight-tested* without the use of wind tunnels. Design of the structures and flight simulations were accomplished primarily using *computational mechanics*.

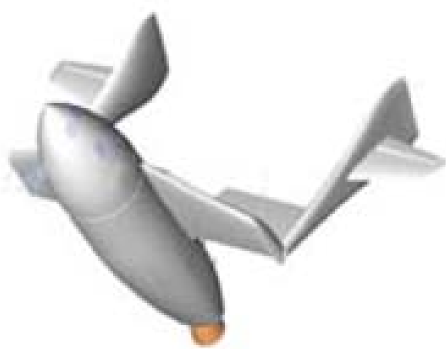

**Figure 6[13]. Feathered configuration of SpaceShipOne during reentry.**

**Commercial Airliners:** Other examples of the progress being made with composites are in the commercial airline industry. Boeing's 787 Dreamliner (Fig. 7) is an ultra light composite airliner.
The composite structure results in 20% less fuel per seat mile as compared with other planes its size. This substantial increase in fuel efficiency is having a significant impact on Boeing's sales of commercial airliners.

Boeing also expects that passengers will notice a significant improvement in comfort due to the higher level of humidity and pressure that can be maintained inside the airliner as a result of the improved thermal insulating properties and higher strength of composites as compared to metals.

**Figure 7[14]. Boeing 787 Dreamliner.**

Whereas Boeing had lost considerable market share to Airbus over the past decade or more, new, lightweight composite planes are reversing that trend. The Boeing 777 typically outsells its European counterpart ten to one, and sales of Boeing's 787 Dreamliner are outpacing Airbus's A380 by a wide margin. The 250 passenger 787 Dreamliner can fly nonstop from Los Angeles to Sydney resulting in additional savings of time and labor during a stopover.

These advances using composite materials are helping the U. S. return to a more competitive position in the sale of commercial airliners. The once-dominant U.S. position in worldwide airliner sales plummeted in the last quarter of the 20$^{th}$ century, but the U.S. share of sales is now moving back above fifty percent largely because of Boeing's composite planes. This is having a significant impact on the U.S. trade deficit, jobs in the United States, and the development of engineering expertise in the United States.

**Unmanned Aerial Vehicles:** A quite different example of the leading-edge use of advanced composites is their application to unmanned aerial vehicles (UAV). The military and NOAA (National Oceanic & Atmospheric Administration) use these high-altitude, longendurance, unmanned aircraft for military reconnaissance and a variety of surveillance activities.

**Figure 8[15]. Lockheed Martin Polecat.**

NOAA conducts oceanic and atmospheric research, climate research, marine sanctuary mapping and enforcement, nautical charting, and fisheries assessment and enforcement using UAVs. Most of the missions for which UAVs are used would be too dangerous, too expensive, or too impractical for manned flight. As with the advanced commercial planes and spacecraft, it is the use of composite materials that makes these missions possible. Thus, composites play a significant role in the study of climate change and global warming through the use of composite UAVs.

One example of a high-flying, stealthy UAV is the "Polecat" (Fig. 6) made by Lockheed Martin. It has a 90-foot wingspan and a tailless design; it looks like a smaller version of the stealth B-2 bomber. The drone is made of 90% composite materials and consists of only 200 parts that are adhesively bonded together rather than riveted. This significantly reduces the labor cost and improves the stealth character.

The examples cited above, while dramatic, are limited to the aerospace field. There are numerous other fields where composites are having far-reaching impact. The fields include but are not limited to: energy generation and conservation, military applications for use on land, sea and air, prosthetic body parts, nanotechnology, corrosion-resistant structures, and more efficient manufacturing capability.

**Transportation Systems:** Essentially all land, sea and air based transportation vehicles (automobiles, trucks, trains, boats, and ships) now employ composite materials to reduce structural weight, improve fuel efficiency, reduce emissions, and provide more damage tolerant, safer structures. Fuel consumption is halved when the weight of a vehicle is cut in half. Accordingly, of the 4 billion pounds of composites shipped in the US in 2004, roughly 43% was used in transportation vehicles. Reducing the weight of trucks, for instance, allows the transport of more goods with less fuel and emissions, and reduces wear and tear on the nation's roadways and bridges.

A specific example of this type of energy conservation is the hybrid automobile that is rapidly gaining acceptance as a vehicle of choice. Improving fuel efficiency in transportation systems and the development of composite-based renewable energy systems has the potential to result in a significant decrease in the nation's dependence on imported oil.

Many opportunities exist for the expanded use of composites in a wide variety of applications. Indeed, many applications are yet to be recognized or discovered. While significant advances have been made with composites in the past half-century, only additional scientific research aimed at improved method for modeling the interaction between the various constituents of a composite and predicting its response when subjected to a complex thermal-mechanical-chemical load history will result in the full potential of these materials. Manufacturing and material costs must be reduced, recycling methods must be developed, and design methods must be improved.

**Renewable Energy:** Large turbines (Fig. 9) used to harvest renewable energy from the wind have blades made of fibrous composite materials. Composites are critically important in the economic viability of wind turbines because of their light weight and high strength and stiffness. With these essential material attributes, composites enable wind turbines to be made more efficient and to last longer.

Ongoing improvements in materials and manufacturing technologies promise a wider use of wind turbines in the future. This will help to facilitate meeting society's energy requirements with less detrimental impact on the environment as well as less dependence on the limited supply of oil.

**Figure 9[16]. Wind turbines. Generating renewable energy**

**Infrastructure:** Composite materials are playing a key role in the rejuvenation of the nation's building and roadway infrastructure (e.g. Ref [17]). Following the great loss of life and property in the 1994 Northridge, California earthquake, for example, thin sheets of fibrous composite materials were applied like structural wallpaper to legions of concrete and masonry buildings, bridges, and elevated roadways in earthquake-prone areas of the nation in an effort to prevent such a catastrophe from happening again.

Similarly, with roughly a quarter of the nation's 600 thousand roadway bridges considered structurally deficient or functionally obsolete, and replacement costs measured in hundreds of billions of dollars, and immeasurable inconvenience to drivers, externally-applied composite reinforcements have emerged as the most attractive means of keeping these bridges in service at their full load rating. The fatigue crack related failure of the I-35W bridge in Minneapolis highlights the advantage of composites that do not exhibit fatigue failures.

Compared to traditional repair materials such as steel plates that require heavy scaffolding and lifting equipment to apply the materials to a structure, light-weight composites allow the rehabilitation work to be quickly done by hand, thus lowering labor costs and traffic congestion. Figure 10 demonstrates the application of carbon fiber composite wraps to provide additional support for a column supporting a superstructure.


**Figure 10[18] Carbon fiber jacketing of a bridge column.**

Composites have the additional advantage of resistance to corrosion by exposure to salt such as in marine environments and northern climates where de-icing agents are commonly used in winter. While much success has been recently obtained in using composite materials to rehabilitate and upgrade civil structures, additional research needs are evident. Improving our ability to predict the long-term performance of the material and the life cycle costs, developing standards and codes, and developing new methods for incorporating composites into infrastructures that better meet the needs of society are needed.

**Biomedical:** Possibly the most intriguing example of how the use of composites can result in a structure that has exceptional capabilities is the human body. The human body is made up of a wide variety of components, including bone, muscle, tendons, blood vessels, lungs, skin and nerve cells, to mention a few (e.g. Ref [19]). Each of these components is, in turn, made of cells and interwoven fibers, typically in a layered or laminated tubular structure.

Figure 11 shows the fibrous nature of a portion of the human body. The interaction of these different constituents is critical to the performance of the body, and composite mechanics offers the means of analyzing and simulating their interactions.

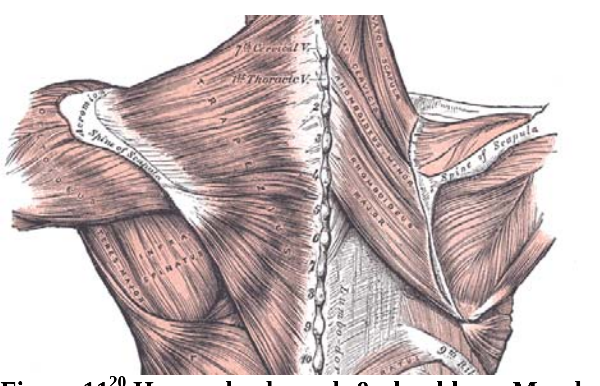

**Figure 11[20] Human back, neck & shoulders. Muscles connecting the upper extremity to the vertebral column.**

**Manufacturing:** Ongoing challenges in the manufacture of composites include the further reduction of cost, the development of polymeric matrix materials that emit less airborne pollutants during manufacture, the development of resins and fibers based on renewable resources such as plants, the development of recycling methods and the development of materials that do not require the use of an autoclave for fabrication.

**Nanocomposites:** New generations of composites incorporating heterogeneity at multiple scales, such as fibers and nano-sized particles, are attracting much interest on account of the interesting properties that arise due to the "nano-effect" (e.g. Ref [21]). These effects are often surprising in that they cannot be predicted based on our understanding of material behavior at large length scales. For instance, as the size of the reinforcement approaches the size of polymeric molecules, the reinforcement becomes actually part of the molecular structure of the polymer, resulting in startling benefits in mechanical, electrical, thermal, and optical performance. Modeling such behavior will require interdisciplinary approaches involving mechanics, materials science, chemistry, and physics.

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***Acknowledgements:***

*The photo at the top of the title page is from Flesher, N. D. & Herakovich, C. T., Damage Evolution in Stiffened Composite Structures Subjected to Variable Loadings. It represents a combination of the two branches of mechanics discussed in this report. It is a finite element representation of the out-of-plan displacements of a stiffened fibrous composite panel when subjected to a combination of thermal and shear loading. This report was reviewed and approved by a subcommittee of the U. S. National Committee on Theoretical and Applied Mechanics.*