3-D Biological Shape, Size and Form Computation

Drs. Mona E. McAlarney, Dentistry and Gautam Dasgupta, Engineering
Columbia University, New York, NY

This multi-disciplinary exploratory research will focus on a new genre of numerical methods accompanied by biological validation to quantify differences in *form (size and shape)* over time and/or under varying conditions including across different populations. This research will enable the best utilization of imaging/digitizing technologies. Surface profiling (outline and coordinate data collection) has been rapidly advancing in 3-D: via PET, NMR, and CAT, along with edge detection and 3-D reconstruction algorithms. However, the numerical quantification of form differences is inadequate, especially in 3-D. Anticipated results will aid in design and/or analysis of biological and/or prosthetic structures. Subsequently, full proposals will be submitted to NSF/NIH for diverse applications in: 1) growth and development analysis, 2) clinical studies, 3) biochemical/electrical activity monitoring, 4) physical anthropology (taxonomy and phylogeny), 5) image analysis, 6) prosthetics, 7) identifying mechanical, thermal or other properties that vary with cell and tissue forms, 8) molecular biology.

Form differences reveal the underlying dynamics. Novel theoretical and numerical algorithms will be investigated here for morphometric quantification. These results will detect regions of atypical morphometrics; histological and/or biomolecular procedures can subsequently follow. In practical clinical studies form difference becomes central to diagnosis, treatment planning, and prognosis, where treatment modalities can be compared. Macromolecular tertiary structure is crucial in molecular biology where differences in form affect activity. Form difference guides design, manufacture, and quality control, in prosthetics, as well as in-vivo changes e.g., wear, mechanical response, and solubility. Thermo-mechanical properties of complex tissues are not directly assessed easily but can be estimated from form differences and applied "forces." Associated finite element and boundary element formulations with stochasticity, will be initiated here for biological systems which are not completely deterministic. A method to quantify exactly the energy due to 3-D form changes in arbitrary geometrical bodies has not yet been formulated. A theoretical scheme for the analytical evaluation of total energy will be undertaken here. At this stage of concept development computer algebra systems, e.g., Mathematica and Matlab, rather than FORTRAN and C, will be used. In subsequent multiyear projects efficient code will be written in C++.

The proposed algorithms are tensorial. Displacement derivative tensors (rate of change of displacement with position) will be constructed from measured differences between the surfaces. Various morphometric parameters, such as size, shape and elongation ratios, as well as maximum elongation direction will be calculated from the tensor eigenvalues and vectors. Unlike traditional heuristic methods, tensorial morphometric analysis provides: 1) both magnitude and direction of form change, 2) results which can be calculated at any point on the surface or within the domain, 3) separation of size and shape changes, and 4) results which are independent of the coordinate system. Results are intuitively visualized via graphic depiction.

Two algorithms for 3-D objects and/or patterns will be developed. The first for structures that have a sufficient number of homologous points (landmarks.) The surface will be tessellated into convex polygons. The displacements between the structures will be described by rational algebraic polynomials (division of two polynomials) interpolating (shape) functions. Form difference variation will be computed as displacement derivatives germane to finite element kinematics. The second pertains to most biological/prosthetic structures, with no or few landmarks. Smooth displacements will be modeled by the Laplace (potential) equation. In this boundary element formulation the available Green's functions will lead to the size and shape change results. "Mean" form statistics will be employed for cases with and without landmarks.

Both landmarks and non-landmark algorithms were extensively scrutinized in 2-D. The numerical results equaled known analytical values for shape changes of pure shear and dilatation. Furthermore, landmark method results of craniofacial rat growth and denture anchor fabrication matched known biological and materials properties, respectively. The non-landmark technique reproduced known growth processes for prenatal rat eyes. Both techniques are numerically stable.

It is not possible to extend some algorithms to 3-D. The anticipated methodology will circumvent currently available techniques such as: 1) landmark interpolating functions, 2) development of homologous patches on the surfaces of non-landmark structures, 3) elliptical Fourier analysis surface fitting routine or another appropriate routine, 4) "mean" form algorithms. Development of these numerical packages for differential tensors to objectively describe any shape/size difference will significantly impact biological and clinical sciences due to their versatile invariant nature.