On-going Research Activities

1. **Exploiting Multi-Core/Hybrid Parallelism** (Elise De Doncker, John Kapenga)

With the emergence of multi-core processors and graphics processing chips, a computer cluster provides for parallelism on multiple levels. It is not yet well-understood how to assess and harvest increased parallel performance for various applications at hand. This results in new programming challenges and the development of tools to exploit hybrid parallelism in systems with multi- and many-core nodes.

2. **Computational Orthopedic Biomechanics** (Peter Gustafson)

Multi-scale analytical methods have not been widely used for orthopedic biomechanics (for some examples see [1][2]). Since the underlying tissue mechanics are stochastic in nature and are driven by physics that span multiple scales, multi-scale stochastic methods may yield significant improvements in model accuracy and human understanding. Significant computational resources are required to produce these outcomes.

Advances in the field of multiple-scale biomechanics will have positive impact on the quality of life of the aging population, realized by advances in orthopedic implants and other medical devices. An improved understanding of the pathology of orthopedic diseases and orthopedic trauma is an additional benefit.

3. **High-Resolution Computational Fluid Dynamics** (William W. Liou)

Detailed understanding of continuum turbulence can be developed using large-eddy simulations (LES) and direct numerical simulations (DNS). These numerical simulation techniques can faithfully represent turbulence physics in a wide range of characteristic scales and provide a tremendous opportunity to simulate and fully resolve many types of engineering turbulent flows. A DNS or LES simulation of a turbulent flow, especially that of engineering interest, requires a large amount of computer resources in both memory and speed. This includes turbulent flows of very large Reynolds numbers, typically found around platforms of interest to the US Department of Defense.

Unsteady flows around flapping wings of, for example, birds and aircraft with flow control, are complex in physics and their simulations demand a time-accurate representation of the entire flow fields at all time. The proposed acquisition of an HPC computer cluster is ideally suited for high-speed, parallel DNS and LES simulations, which are generally believed to play a key role in the further advancement of the understanding of fluid turbulence.

4. **Computation of Feynman Loop Integrals by Iterated Adaptive Integration** (E. de Doncker)

Feynman loop integrals, occurring in high energy physics perturbation calculations, contribute corrections to the scattering amplitude and the cross section for the collision of elementary particles. In general, very large sets of these (multivariate) integrals may be required.

Multivariate integration may be very computational intensive, especially when the integrand exhibits a singularity within the integration domain. Loop integrals are often divergent. We use numerical extrapolation in order to eliminate terms from the asymptotic error expansion (as a parameter in the integrand function tends to zero) [3]. This requires evaluating an increasingly difficult sequence of integral approximations. The calculations are performed using a process of *iterated* adaptive integration, where suitable one- and multi-dimensional integration methods can be combined in different coordinate directions. The integration and extrapolation methods have been adopted in the GRACE system [4], with the purpose of further automating cross section calculations. In order to support the calculations of Feynman loop diagrams, we plan to modify and extend the parallel software package ParInt [5] developed at WMU, by adding a procedure of iterated integration and extrapolation methods in a transparant way.

4. **Parallel Computation of Flexible Body Aerodynamics** (Dewei Qi)

A flexible particle lattice Boltzmann method (FPLBM) for direct simulations of flexible solid structures in a low Reynolds number flow has been developed and validated for a flexible membrane in a fluid [6]. It is demonstrated that this method can be used in flexible body aerodynamics. The approach is based on a lattice Boltzmann (LB) simulation and a ball and socket model for a flexible structure. The fluid domain is dealt with using the lattice Boltzmann equation, which is equivalent to solving Navier-Stokes equations on a massive parallel computer or cluster.

The following tasks are at hand: (1) We will conduct a set of computational experiments on flapping membrane wings at different Reynolds numbers and the results will be compared directly with experimental and theoretical results. (2) We will apply the flexible particle method to optimize the flexibility in the chord direction. The simulation results may provide more useful information for controlling separation using

flexible wings. (3) In future work we will investigate whether we are able to simulate a twisting wing with a smaller attack angle at the wing tip when the equilibrium twisting angle is nonzero. (4) Flag-in-the-wind problems with active control are not difficult to study using the same method. The active control can be easily realized by prescribing one or several membrane segments, and the motion of other membrane segments could be obtained from simulations.

6. **Uses of Multiprocessor Cluster Power in the PCI department** (Paul Dan Fleming)
The following projects are of interest: (1) Simulation of paper coating pigment packing and morphology for different particle shapes. (2) Simulation of binder polymer and pigment interaction. The binder polymer not only assists in film formation and holding the pigment particles, but also helps adhere the coating to the base paper. This effort can effectively utilize molecular dynamics simulations, which are known to make effective use of multiple processors. (3) Simulation of packing of ink pigments with coating pigments for printing on paper. The ink layer may increase the gloss relative to the paper or it may decrease it. These simulations would elucidate the mechanisms of ink gloss over a glossy or matte coated paper. (4) Simulation of multiple functional layers in printed electronics. Printing functioning electronic devices not only depends on the smoothness of the substrate, but also on the smoothness of the previously printed functional layer. Smoothness of intermediate layers not only improves the performance of the printed devices, but also makes for more cost effective material use.

7. **Supercomputing for Chemical and Biological Problems** (Yirong Mo)
Yirong Mo of the Chemistry Department has primary research interests in the development of novel theoretical and computational methods and the application of these methods to chemical and biological problems. The following major research lines in his lab require high-performance computer facilities.

The first project is an integrated collaborative effort by a team of experimentalists and computational chemists with the attempt to elucidate the reaction mechanism catalyzed by DXR. Transition state stabilization is the hallmark of enzymatic catalysis. The enormous catalytic power of an enzyme lies in that it binds to and stabilizes the transition state in preference to any other molecular species. The proposed research will bring a giant leap in our understanding of the catalytic mechanism of DXR. The proposed research is not only of fundamental significance for the understanding of DXR catalysis but is also valuable for the development of antibiotics, antimalarial drugs, and herbicides.

The second project integrates the theoretical development and the computational applications that can bridge the experimental phenomena and conventional chemical concepts and theories. The proposed general BLW method, which can be regarded as the simplest variant of the VB theory, uniquely combines the characteristics of both VB and MO theories, and can be implemented and employed efficiently. Applications of this general BLW method can provide novel understanding and interpretation of experimental and accurate MO results in terms of conventional chemical concepts at the computational costs of the MO theory.

---

[1] Marco Viceconti. Multiscale modelling and team science: the future of orthopaedic biomechanics. *Journal of Foot and Ankle Research*, 1(Suppl 1):K6 (2008)

[2] Marco Viceconti, Fulvia Taddei, Serge Van Sint Jan, Alberto Leardini, Luca Cristofolini, Susanna Stea, Fabio Baruffaldi, and Massimiliano Baleani. Multiscale modelling of the skeleton for the prediction of the risk of fracture. *Clin Biomech (Bristol, Avon)*, 23, 7 (2008), 845–852

[3] Elise de Doncker, Junpei Fujimoto, Yoshimitzu Shimizu and Fukuko Yuasa. Computation of loop integrals using extrapolation. *Computer Physics Communications* 159 (2004), 145-156.

[4] GRACE/SUSY (GRACE v2.2.0). Available from http://minami-home.kek.jp

[5] ParInt © 1999 *Library of Congress*. E. de Doncker, A. Gupta, A. Genz and R. Zanny

[6] Dewei Qi, Direct simulations of flexible cylindrical fiber suspensions in finite Reynolds number flow, *J. Chem. Phys. 125, 114901 (2006)*