Matrix Computations & Scientific Computing Seminar

Organizer: James Demmel & Ming Gu

Wednesday, 12:10–1:00pm, 380 Soda

Feb. 1   **Chris Rycroft**, UCB and LBL
Application of the Voronoi tessellation for high-throughput analysis of crystalline porous materials

Crystalline porous materials, such as zeolites, contain complex networks of void channels that are exploited in many industrial applications. Since the 1950s, they have been employed in common applications such as chemical catalysts and water softeners, and more recently there has been interest their use for new technologies such as carbon capture and storage. A key requirement for the success of any nanoporous material is that the chemical composition and pore topology must be optimal for a given application. However, this is a difficult task, since the number of possible pore topologies is extremely large: thousands of materials have been already been synthesized, and databases of millions of hypothetical structures are available.

We have developed tools for rapid screening of these large databases to automatically select materials whose pore topology may make them most appropriate for a given application. Many of the methods are based on computing the Voronoi network, which provides a map of void channels in a given structure. This is carried out using the free software library Voro++, which has been modified to properly account for three-dimensional non-orthogonal periodic boundary conditions.