

## **Software challenges in scientific computing at the dusk of Moore's Law**

**Thomas C. Schulthess**

Today's scientific computing systems are massively parallel processing arrays with multi-threaded compute nodes that have complex memory hierarchies. In some cases, compute nodes have heterogeneous memory and compute resources, such as GPU accelerators or high-bandwidth/non-volatile memory. This diversity of architectures will further increase, as we approach the end of Moore's Law. Scientific application software has to be portable across all these architectures and at the same time perform optimally on each individually. We will discuss software strategies that allow us to tackle this challenge while maintaining high productivity of scientists who have to use and further develop application software. A specific example will be given for electronic structure codes.