Survey of Out-of-Core Algorithms in Numerical Linear Algebra

Sivan Toledo

Abstract

Algorithms that solve problems too large to fit within the main memory of the computer have been used in numerical linear algebra since the early 1950s. Such algorithms, known as out-of-core algorithms, store large data structures on disks (and other secondary memory devices in the past). The talk will survey out-of-core algorithms in numerical linear algebra. I will discuss theoretical and practical design considerations, describe the algorithms themselves, and sketch the history of this field.

I will describe out-of-core algorithms in the following areas:

- dense linear algebra (linear solvers, least squares, eigenvalues),
- sparse direct linear and least-squares solvers,
- sparse iterative solvers,
- fast Fourier transforms, and
- n-body solvers.

The specific algorithms will be described in the context of several fundamental theoretical and practical issues. I will introduce these issues in the beginning of the talk and will revisit them as we investigate specific algorithms. These issues are:

- architectural and economic issues for out-of-core algorithms,
- scheduling for data reuse and Hong-Kung-type bounds on data reuse,
- scheduling and data layout for input/output of large blocks,
- transformations that enable efficient schedules,
- methodologies for designing out-of-core algorithms, such as block and partitioned algorithms,
- cost measures that have been used in the literature, such as the number of passes over the data, the level-3 fraction, and asymptotic data-reuse bounds.

- similarities and differences between out-of-core and other environments that favor data reuse, such as caches and distributed-memory parallel machines.

I will also comment on the history of out-of-core algorithms in numerical linear algebra. My comments are designed to elucidate two interesting phenomena. I will explain why some out-of-core algorithms become obsolete, and why other algorithms are forgotten without becoming obsolete and are rediscovered later. For example, I will explain why a certain class of out-of-core iterative linear solvers became obsolete, and I will show that blocked matrix multiplication dates back to 1951, but was largely forgotten and then rediscovered.