Building a better solver: software engineering aspects of high-performance scientific computing. II.

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ABSTRACT. Numerical solution of large systems of linear and nonlinear algebraic equations is at the heart of most problems in scientific computing. As we attempt to produce simulations of ever greater size and complexity, solver algorithms often must be tailored to exploit the structure of a particular problem. In such algorithms, each solve may have numerous intermediate data structures and operations – including other solves on subproblems – that need to be coordinated. Furthermore, as simulations are being run on increasingly complex computer architectures we need to tune our programs to those architectures all the while maintaining the flexibility needed for use in tailored solvers.

In this series of talks I'll outline some of the challenges for programming solver algorithms. I'll use as a case study the deceptively simple concept of programming operations on vectors, and show how we can design software that is easy to understand and use without sacrificing performance and flexibility. Along the way you'll meet some nifty programming tricks such as factory patterns, expression templates, and lazy evaluation. I'll introduce a new software toolkit, Playa ("Painless Linear Algebra"), that embodies these ideas.