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"Mathematical Programming without Derivatives – Exacting Penalties is a Good Thing"

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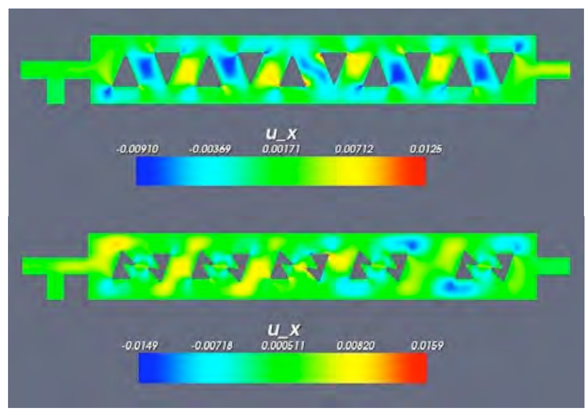
Summary

Optimization is often daunting to engineers and scientists because it involves complicated derivative calculations and the software is hard to use. We have developed robust derivative-free methods and software that are easy to use, run efficiently in parallel (even when the scientist's code is not parallel), and are mathematically proven to converge. Nonlinear programming problems are solved using so-called penalty methods when nonlinear constraints are present.

Our focus is on solving real-world optimization problems from science and engineering – the types of problems that are based on complicated (perhaps even stochastic) simulations that are expensive and do not have any derivative information. Few optimization methods or codes can solve such problems and fewer still can do so when constraints are involved. We have designed a parallel and *asynchronous* derivative-free optimization method that reliably and robustly solves nonlinear programming problems without using derivatives.

Application pay-off has been immediate. Using APPSPACK's support for linear constraints, Sandia engineers have been able to:

1. Reduce vehicle emissions by designing a lean NOx trap using the commercial CHEMKIN simulator.
2. Improve detection of chemical agents such as anthrax by finding an optimal configuration for a microfluidic mixing device.



Design of a microfluidic mixing device for chemical detection before and after APPSPACK optimization.

Over the past two years, we have extended our methods to handle linear and nonlinear constraints. This advancement means that more complicated nonlinear programming problems can now be solved.

The search pattern that is used to select trial points for evaluation in the simulator is adjusted automatically in the case of linear constraints. The best methods for handling nonlinear are so-called *penalty methods*

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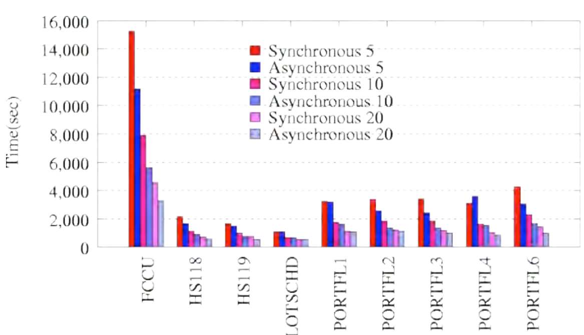
which add a penalty term in the objective function for violated constraints. The key is choosing the type and degree of penalization. With a focus on getting a *good, feasible* solution quickly (~1000 evaluations) rather than a perfect solution using orders of magnitudes more evaluations, we have found that so-called smoothed-exact penalty functions are ideal. These methods have not received much attention in recent years but are in fact extremely powerful.

With all these changes, the key to our success is still allowing different simulations to run independently and asynchronously. Time is wasted on supercomputers for synchronization, but our methods fix this problem by efficiently using of available resources. Our asynchronous implementation is faster than a synchronous one, even for problems with constraints; see figure below.



Numerical results on 9 linearly constrained problems; our asynchronous method (blue) is faster than synchronous (red) on the same number of processors (5,10,20).

Moreover, our convergence theory proves that these methods converge to a constrained stationary point – i.e., a true mathematical solution that is as good as would be achieved using derivative-based methods (if that were an option).

All these methods are implemented in the code APPSPACK, freely downloadable from http://software.sandia.gov/appspack under the terms of the GNU L-GPL license. APPSPACK runs in parallel using MPI, and it interfaces with the simulation via file I/O, meaning that the simulation can be written any language. This is the only derivative-free code that supports linear and nonlinear constraints.

In the past year, our publications appeared in *ACM Trans. on Math. Software* and *SIAM J. Optimization*. We submitted two papers to *SIAM J. Scientific Computing*. We are active in the community, presenting invited lectures at scientific meetings.

We are currently in the process of adding support for *global optimization* using hybrid methods that combine global and local methods.

Our work with applications has been aided by our colleagues at Sandia National Laboratories. Our theoretical work has been in collaboration with Prof. Virginia Torczon and Prof. R. Michael Lewis at the College of William and Mary in Virginia. The development of the APPSPACK software has also been partly supported by the NNSA.

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