Improving Optimization Performance with Parallel Computing

Engineers, scientists, and financial analysts frequently use optimization methods to solve computationally expensive problems such as smoothing the large computational meshes used in fluid dynamic simulations, performing image registration, or analyzing high-dimensional financial portfolios. However, computing a solution can take anywhere from hours to days.

Products Used

- MATLAB®
- Simulink®
- Optimization Toolbox™
- Statistics Toolbox™
- Parallel Computing Toolbox™
- MATLAB Distributed Computing Server™

Parallel computing techniques can help reduce the time it takes to reach a solution. To derive the full benefits of parallelization, it is important to choose an approach that is appropriate for the optimization problem.

This article describes two ways to use the inherent parallelism in optimization problems to reduce the time to solution. The first example solves a mathematical problem using the parallel computing option in Optimization Toolbox™, and requires no code modification. The second, a practical engineering optimization problem, requires a single-line change in code. Both examples use Parallel Computing Toolbox™ and MATLAB Distributed Computing Server™ to automate and manage the parallel computing tasks.

Parallel Optimization with Optimization Toolbox

In a typical optimization, an iterative search procedure is used to find a minimum value of a given function—for example, using a gradient-based algorithm to find a minimum value of the peaks function in MATLAB® (Figure 1).

Gradient estimation is often the most time-consuming computation during optimization. In a single iteration, the optimization solver estimates the local gradient of the function and uses that information to determine the direction of the search and the magnitude of the step to the next point in the search. This process is repeated until

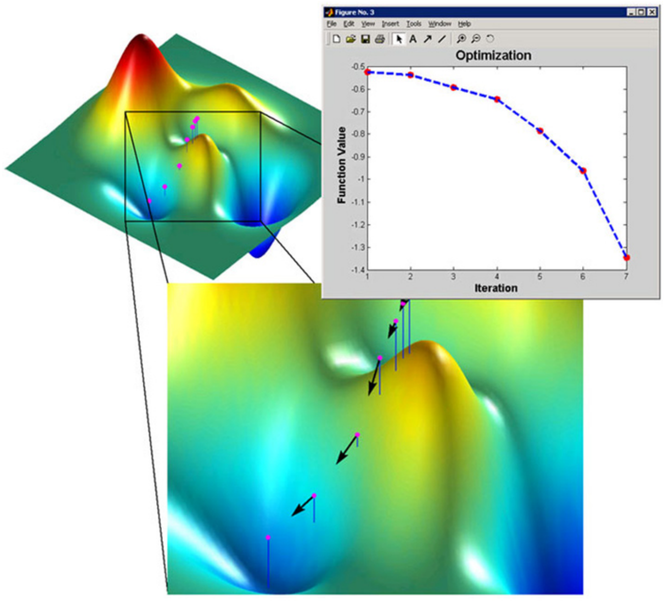


Figure 1. Using a gradient-based optimization solver to search for a minimum value.

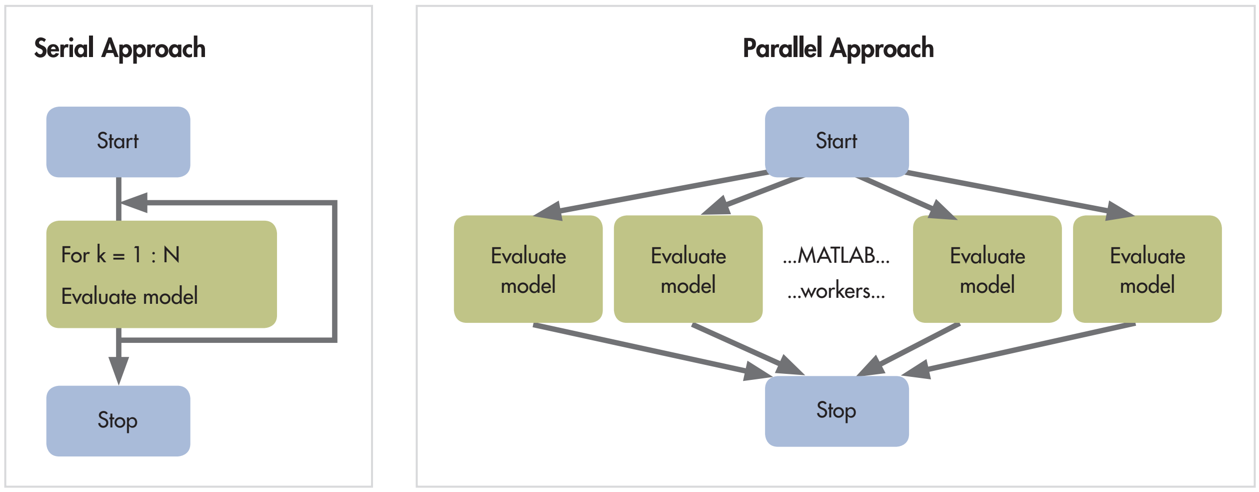


Figure 2. Serial and parallel approaches to gradient estimation.

the solver finds a minimum value or reaches a predefined time or iteration limit.

The gradient estimation step, which is often performed using an approximation method, such as finite differences, requires several function evaluations near the current point. Typically, N function evaluations are required, where N is the number of variables, or the dimensionality of the problem. As N increases, so do the number of function evaluations for each iteration and the time to solution.

Figure 2 shows how you can perform computations in parallel to accelerate gradient estimation. The N function evaluation used to estimate the gradient when performed on a single MATLAB worker would be executed serially.

Whereas in the serial approach the N function evaluations occur one after the other, in the parallel approach the computations are distributed across MATLAB workers, and several function evaluations can occur simultaneously. We can speed up gradient estimation as long as the cost of distributing the function evaluation across multiple workers is less than the execution time of N objective (and constraint) function evaluations. The actual solution time depends on the objective/constraint function execution speed, the computer processing speed, available memory, current load, and network speed.

An ElectroStatics Example[i]

This example illustrates how to formulate and solve an optimization problem in MATLAB. Consider N electrons in a conducting body (Figure 3). The electrons arrange themselves to minimize their potential energy subject to the constraint of lying inside the conducting body. At the minimum

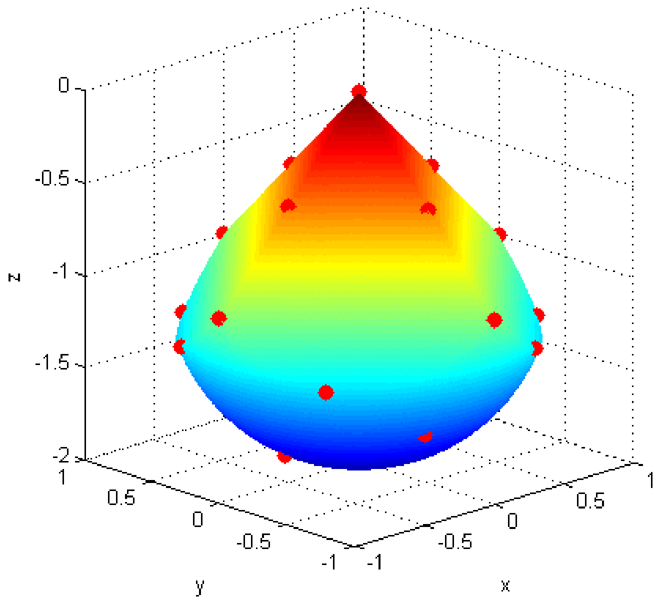


Figure 3. Conducting body and electrons.

[i] Inspired by Dolan, Moré, and Munson, "Benchmarking Optimization Software with COPS 3.0", Argonne National Laboratory Technical Report. ANL/MCS-TM-273, February 2004.

total potential energy, all the electrons lie on the boundary of the body. Because the electrons are indistinguishable, there is no unique minimum for this problem (permuting the electrons in one solution gives another valid solution).

The optimization goal is to minimize the total potential energy of the electrons subject to the constraint that the electrons remain within the conducting body. The objective function, potential energy, is the sum of the inverses of the distances between each electron pair (i,j = 1, 2, 3,… N):

$$energy = \sum_{i<j} \frac{1}{\left| x_i - x_j \right|}$$

The constraints that define the boundary of the conducting body are

$$z \le -|x| - |y|$$

$$x^2 + y^2 + (z+1)^2 \le 1$$

As written, the first inequality is a non-smooth nonlinear constraint because of the absolute values on *x* and *y*. Absolute values can be linearized to simplify the optimization problem. This constraint can be written in linear form as a set of four constraints for each electron, *i*.

$$x_{i,3} - x_{i,1} - x_{i,2} \le 0$$

$$x_{i,3} - x_{i,1} + x_{i,2} \le 0$$

$$x_{i,3} + x_{i,1} - x_{i,2} \le 0$$

$$x_{i,3} + x_{i,1} + x_{i,2} \le 0$$

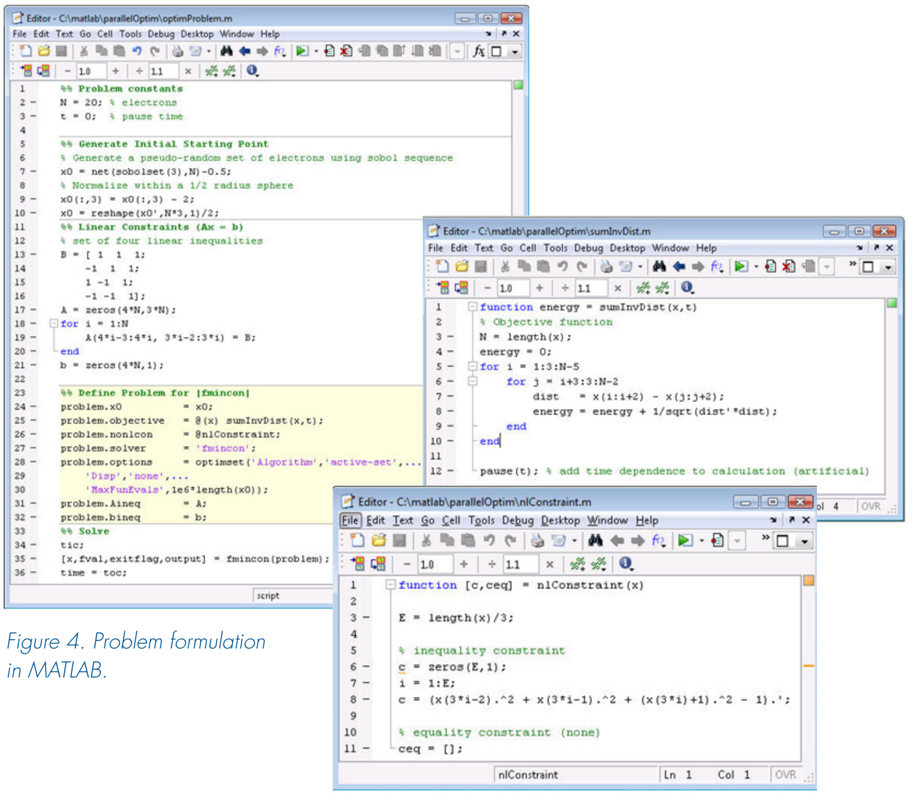
The indices 1, 2, and 3 refer to the *x, y,* and *z* coordinates, respectively.

This problem can be solved with the nonlinear constrained solver `fmincon` in Optimization Toolbox. Figure 4 shows the problem formulation in MATLAB. Note that in defining the objective function, `sumInvDist`, the statement `pause(t)` was added. This changes the time taken to execute `sumInvDist`, letting us determine how the execution time changes the solution time.

We execute the optimization problem on a single MATLAB worker. For convenience, we define speed-up as the ratio of the time it takes to solve the problem on 1 worker relative to the time it takes to solve the same problem on N workers. Thus, for any problem running on a single worker, the speed-up is defined as 1. When the same problem is run on more than one worker, a speed-up greater than one denotes a reduction in solution time and a speed-up less than one denotes an increase.

To use the parallel computing capability in Optimization Toolbox, we change the '`UseParallel`' option from the default, 'Never,' to 'Always', enable the desired number of compute nodes with the `matlabpool` command, and run the optimization solver as before (Figure 5).

This example runs on two workers and is 20% slower than the single-worker case. The evaluation time of N objective and constraint functions is on the order of 0.5 milliseconds. A single evaluation of the objective function and the constraint function takes about 0.5 milliseconds. Because the evaluations take so little time, the overheads associated with farming out data and computations outweigh any gains that are realized by running the code in parallel. As a result,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```
%% Problem constants
N = 20; % electrons
t = 0;  % pause time

%% Generate Initial Starting Point
% Generate a pseudo-random set of electrons using sobol sequence
x0 = net(sobolset(3),N)-0.5;
% Normalize within a 1/2 radius sphere
x0(:,3) = x0(:,3) - 2;
x0 = reshape(x0',N*3,1)/2;
%% Linear Constraints (Ax = b)
% set of four linear inequalities
B = [ 1  1  1;
     -1  1  1;
      1 -1  1;
     -1 -1  1];
A = zeros(4*N,3*N);
for i = 1:N
    A(4*i-3:4*i, 3*i-2:3*i) = B;
end
b = zeros(4*N,1);

%% Define Problem for |fmincon|
problem.x0          = x0;
problem.objective   = @(x) sumInvDist(x,t);
problem.nonlcon     = @nlConstraint;
problem.solver      = 'fmincon';
problem.options     = optimset('Algorithm','active-set',...
    'Disp','none',...
    'MaxFunEvals',1e6*length(x0));
problem.Aineq       = A;
problem.bineq       = b;
%% Solve
tic;
[x,fval,exitflag,output] = fmincon(problem);
time = toc;
```

```
function energy = sumInvDist(x,t)
% Objective function
N = length(x);
energy = 0;
for i = 1:3:N-5
    for j = i+3:3:N-2
        dist   = x(i:i+2) - x(j:j+2);
        energy = energy + 1/sqrt(dist'*dist);
    end
end

pause(t); % add time dependence to calculation (artificial)
```

```
function [c,ceq] = nlConstraint(x)

E = length(x)/3;

% inequality constraint
c = zeros(E,1);
i = 1:E;
c = (x(3*i-2).^2 + x(3*i-1).^2 + (x(3*i)+1).^2 - 1).';

% equality constraint (none)
ceq = [];
```

Figure 4. Problem formulation in MATLAB.

```
problem.options = optimset(problem.options,'UseParallel','Always');
matlabpool open 2
[x,fval,exitflag,output] = fmincon(problem);
```

Figure 5. Running the optimizaton solver using the parallel computing capability in Optimization Toolbox.

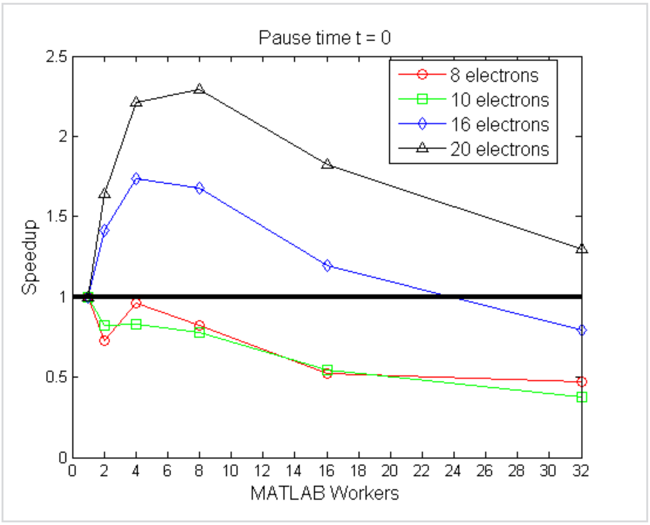


Figure 6a. Results for pause time t = 0 seconds.

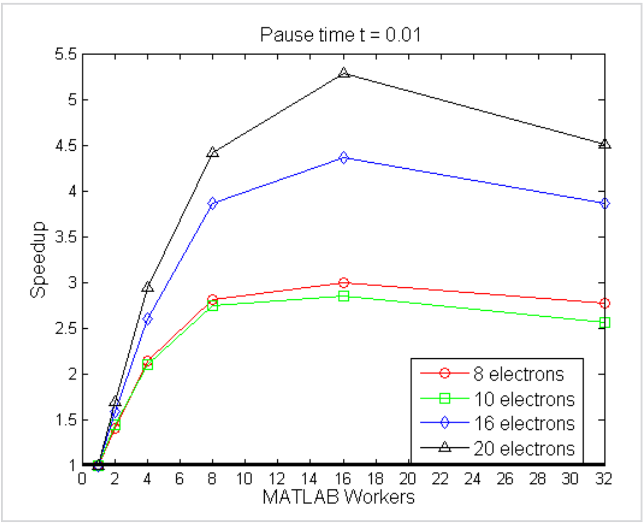


Figure 6b. Results for pause time t = 0.01 seconds.

distributing computations to run in parallel is slower than running the problem serially.

This example shows that for optimization problems to benefit from running the computations in parallel, the cost associated with the function evaluations with gradient estimation must be greater than the overhead costs associated with data and code transfer.

To further understand the trade-offs associated with the objective function execution time, number of MATLAB workers, and number of variables (electrons), we ran this problem with a pause time (t) ranging from 0 to 0.4 seconds, different workers from 1 to 32, and number of electrons ranging from 8 to 20. Figures 6a and 6b show the results plotted for t = 0 and 0.1 seconds, respectively.

Figure 6a shows how the number of electrons changes the speed-up. For 8 and 10 electrons, the overhead cost of more workers reduced the speed-up. For 16 electrons, the overhead cost fell below the function evaluation cost, and we saw a positive effect on the speed-up for most workers. The average time to evaluate one objective function was on the order of 1 millisecond on a single worker. The maximum speed-up occurred at around 8 workers. Increasing the number of workers increased the communication overhead and eventually eliminated the benefit of using parallel computing.

Figure 6b shows how the results change when the objective function evaluation time significantly exceeds the overhead costs. A rapid increase in speed-up is again observed around 8 workers. Notice that the maximum reductions in the curve for the 8-electron case and the 16-electron case are 8 workers and 16 workers, respectively. This increase is a result of balancing the number of parallel computations that can be performed with the same number of workers. For the 8-electron case, 8 workers resulted in the greatest increase. A similar trend is seen for the 16-electron case.

User-Defined Parallel Optimization Problem

As we have seen, the time required to evaluate the objective strongly influences the solution time. Therefore, one of the approaches we can take is to look for parallelism within the objective function and the constraint function—that is, to parallelize the objective or the constraint function.

We will take this approach by distributing computations within the objective function for the problem shown in Figure 7. The

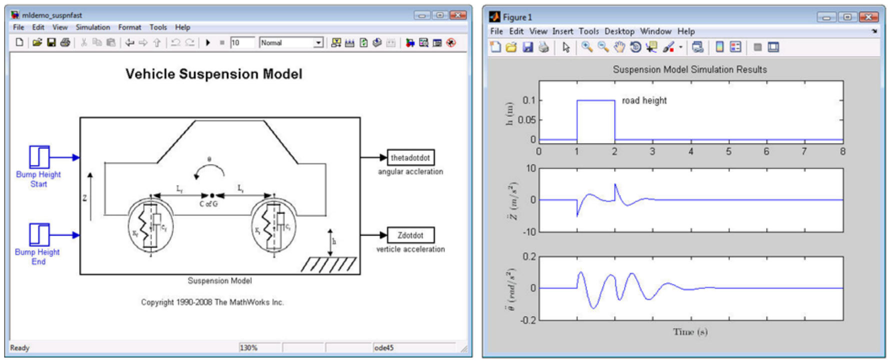


Figure 7. Vehicle suspension model and simulation results for an empty vehicle.

goal of this problem is to design a suspension system that minimizes the discomfort the driver would experience when traveling over a bump in the road. At the same time, we must account for uncertainty in the mass of the driver, passengers, and trunk loadings. We can modify the four parameters that define the front and rear suspension system stiffness and damping rate: *kf, kr, cf, cr*. The masses of the driver, passengers, and trunk loadings are uncertain and have a normal distribution assigned to them.

A Monte-Carlo simulation is performed to capture the different vehicle loadings. The model outputs are angular acceleration about the center of gravity (`thetadotdot`, $\ddot{\theta}$) and vertical acceleration (`zdotdot`, $\ddot{z}$).

The objective function, `myCostFcnRR`, contains a Monte-Carlo simulation used to evaluate the mean and standard deviation of acceleration that the passengers would experience (Figure 8). The goal is to minimize the mean and standard deviations.

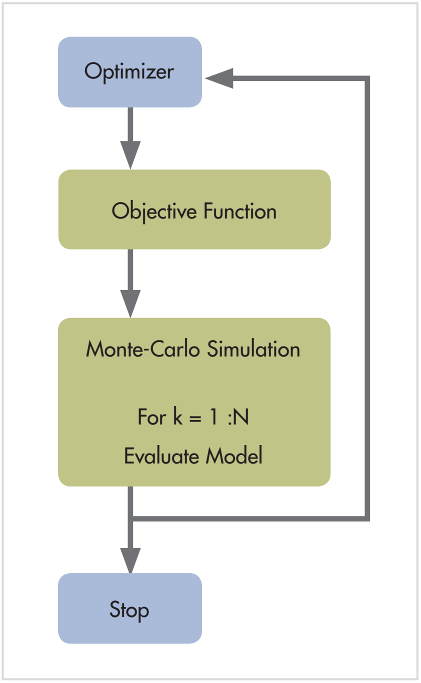
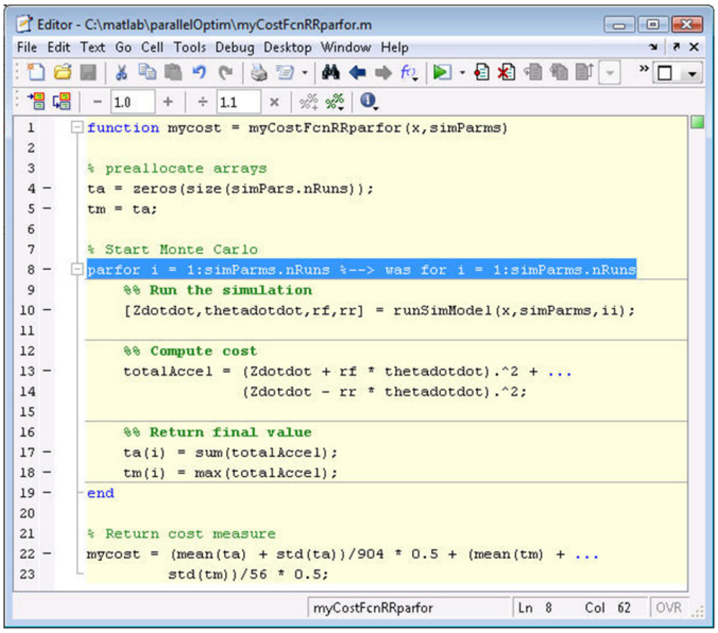


Figure 8. Objective function used to run a Monte-Carlo simulation within the optimization process.

In a Monte-Carlo simulation, each run is independent and therefore can benefit from parallel computation. To convert the problem from serial to parallel, we simply replace the `for` loop construct with the `parfor` (parallel `for` loop) construct (Figure 9). The objective statements inside the `parfor` loop can then run in parallel, speeding up the objective function evaluation time.

The optimization problem was run for three different values of `nRuns`, the number of points to evaluate in the Monte-Carlo simulation. The results show that parallelizing the objective function yielded substantial performance gains (Figure 10).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```
function mycost = myCostFcnRRparfor(x,simParms)

% preallocate arrays
ta = zeros(size(simPars.nRuns));
tm = ta;

% Start Monte Carlo
parfor i = 1:simParms.nRuns %--> was for i = 1:simParms.nRuns
    %% Run the simulation
    [Zdotdot,thetadotdot,rf,rr] = runSimModel(x,simParms,ii);

    %% Compute cost
    totalAccel = (Zdotdot + rf * thetadotdot).^2 + ...
                 (Zdotdot - rr * thetadotdot).^2;

    %% Return final value
    ta(i) = sum(totalAccel);
    tm(i) = max(totalAccel);
end

% Return cost measure
mycost = (mean(ta) + std(ta))/904 * 0.5 + (mean(tm) + ...
         std(tm))/56 * 0.5;
```

Figure 9. Objective function modified to execute in parallel.

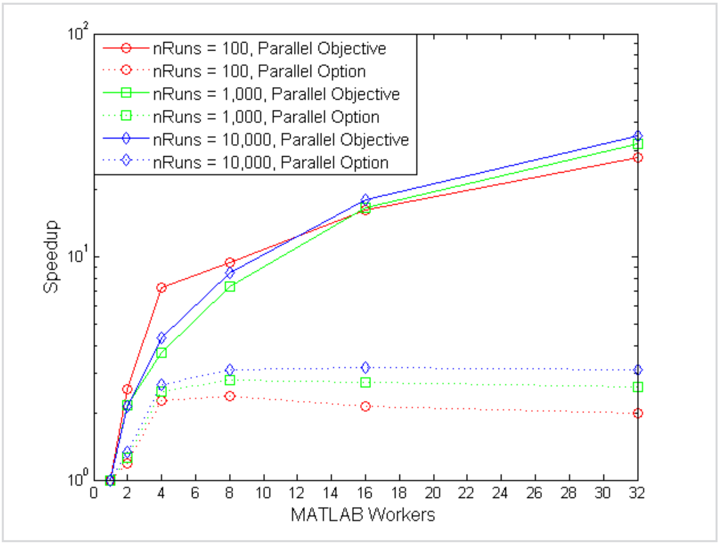

Figure 10. Results for the suspension system design problem.

MATLAB Distributed Computing Server

Computer Setup

8 networked PCs configured with Linux 2.6, 2 dual-core AMD Opeteron 2.59 GHz processors, 3 GB RAM.

Selecting a Parallelization Method

As the results show, it is best to select a parallelization method based upon where computational expense is encountered in the optimization problem. The first example showed that it is possible to see a reduction in performance even after distributing computations if the objective/constraint function execution time does not exceed the communication overhead. For the problem and hardware configuration tested, we would need an execution time of at least one millisecond to see any benefit from parallelizing the problem.

The second example showed that the benefits obtained by performing parallel computations can depend on the problem being solved. Using the parallelism within the objective function—that is, parallelising the objective function itself—resulted in better performance than would have been possible using the parallel computing option in Optimization Toolbox. In this example, the execution time of the objective function was the slowest part of the optimization problem, and speeding up the objective function resulted in the greatest reduction in solution time.

In summary, when selecting a parallelization approach it is important to consider the number of available workers and the execution time of the objective/constraint function relative to overheads associated with distributing computations across multiple workers The built-in support in Optimization Toolbox is beneficial for problems that have objective/constraint functions with execution times greater than network overhead. However, parallelizing the objective/constraint function itself can be a better approach if it is the most expensive step in the optimization problem and can be accelerated by parallelizing the objective function. ■

For More Information

- Designing for Reliability and Robustness. *MATLAB Digest,* January 2008 *www.mathworks.com/company/robustdesign*
- Cleve's Corner: Parallel MATLAB: Multiple Processors and Multiple Cores, *The MathWorks News and Notes,* June 2007. *www.mathworks.com/company/parallelmatlab*