

Block-by-block description of MATLAB code

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1. Setting convergence and stagnation thresholds

Convergence threshold (target residual norm): This value defines when the optimization is considered converged.

```
1 target_residual_norm = 1e-3;
```

Stagnation tolerance: If residual norm does not change significantly (difference less than this value), the algorithm is considered stuck.

```
1 stagnation_tol = 1e17;
```

2. Initialization of initial guess

Initial parameter vector: Pack parameters and fields into a vector.

```
1 x0 = packFieldsAndInterface(fields, params.M
    , params.N, length(params.c_init), params
    .c_init);
```

3. Definition of anonymous residual function

Anonymous function computing residual vector:

```
1 fun = @(x) computeResidualVector(x, params,
    dx, dy, X, Y, x_interface);
```

4. Optimization options

Options for lsqnonlin: - detailed display, - max iterations 100, - function tolerance 1e-6.

```
1 options = optimoptions('lsqnonlin', ...
2 'Display', 'iter-detailed', ...
3 'MaxIterations', 100, ...
4 'FunctionTolerance', 1e-6);
```

5. Initialization for restart loop

Variables to control restarts and residual norms:

```
1      max_restarts = 10;
2      restart_count = 0;
3      resnorm = Inf;
4      previous_resnorm = Inf;
```

6. Restart optimization loop

Run optimization while residual norm is above target and restarts are below maximum:

```
1      while resnorm > target_residual_norm &&
2          restart_count < max_restarts
3          fprintf('Run #d\n', restart_count + 1);
4
5          [x_opt, resnorm, residual, exitflag, output]
6              = lsqnonlin(fun, x0, [], [], options);
7
8          fprintf('resnorm after iteration: %.6e\n',
9              resnorm);
10
11         delta_resnorm = abs(previous_resnorm -
12             resnorm);
13         if delta_resnorm < stagnation_tol
14             fprintf('resnorm change too small:      = %.2e
15                 < %.2e      restart\n', delta_resnorm,
16                 stagnation_tol);
17         end
18
19         previous_resnorm = resnorm;
20         x0 = x_opt;
21         restart_count = restart_count + 1;
22
23         save('optimization_intermediate.mat', 'x0',
24             'resnorm', 'restart_count');
25     end
```

7. Final output

Check if convergence was successful:

```
1      if resnorm <= target_residual_norm
2          fprintf('Convergence achieved: resnorm = %.6
3              e\n', resnorm);
4      else
```

```
4         fprintf('Accuracy not reached after %d\n',  
5         restarts. Final resnorm = %.6e\n',  
         restart_count, resnorm);  
         end
```

8. Unpacking solution

Convert optimized vector back to fields and parameters:

```
1         [fields_opt, c_opt] =  
         unpackFieldsAndInterface(x_opt, params.M,  
         params.N, length(params.c_init));
```