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Modified Sequential Kriging Optimization for Multidisciplinary Complex Product Simulation

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Abstract

Directing to the high cost of computer simulation optimization problem, Kriging surrogate model is widely used to decrease the computation time. Since the sequential Kriging optimization is time consuming, this article extends the expected improvement and put forwards a modified sequential Kriging optimization (MSKO). This method changes the twice optimization problem into once by adding more than one point at the same time. Before re-fitting the Kriging model, the new sample points are verified to ensure that they do not overlap the previous one and the distance between two sample points is not too small. This article presents the double stopping criterion to keep the root mean square error (RMSE) of the final surrogate model at an acceptable level. The example shows that MSKO can approach the global optimization quickly and accurately. MSKO can ensure global optimization no matter where the initial point is. Application of active suspension indicates that the proposed method is effective.

Keywords: surrogate model; Kriging; expected improvement; collaborative simulation; optimization

1. Introduction

Conventional simulation methods are not capable of solving comprehensive product design problem, so multidisciplinary collaborative simulation method emerges as the times require for such complicated engineering simulation problem^[1]. Since the evaluation cost of collaborative simulation is high, surrogate model provides a cheaper but lower-fidelity solution^[2]. Kriging model, one of the surrogate models, is gaining popularity as a way of developing fast approximation system for time-consuming simulations. Due to the challenge of interpolation strategy in Kriging model, this article deals with collaborative simulation and optimization based on Kriging model.

In real-life optimization problems, finding the global maximum or minimum of a function is much more

challenging and has been practically impossible for many problems so far^[3]. With the big difficulties of gradient calculation for complex model, the traditional gradient-based methods are not suitable in this area. In former research, sequential Kriging optimization (SKO) algorithm is used to find the best solution based on Kriging surrogate model while it is time consuming due to its sampling rule, in which only one point with the biggest expected improvement (EI) function will be added in each iteration^[4]. How to design an algorithm to fit the model at an acceptable level with fewer iterations of optimization during global optimization is urgent to solve in SKO^[5]. In order to solve the above problems, we put forward the modified sequential Kriging optimization (MSKO) method with dynamic update criterion during the optimization process.

2. Surrogate Model Based on Kriging

Kriging surrogate model is considered as the best linear unbiased estimation to the real computer model. It is a semi-parametric interpolation technique which estimates the unknown information at one point according to the known information^[6]. Nowadays, it has

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become a popular method for approximating deterministic computer model.

The approximation of original model can be expressed as the following formula under the conditions of multiple inputs and single output^[6-7]:

$$\hat{y}(X) = \sum_{j=1}^k \beta_j f_j(X) + Z(X) = \beta f(X) + Z(X) \quad (1)$$

where $X=[x_1 \ x_2 \ \dots \ x_n]$ is the input, $f_j(X)$ the known polynomial function chosen by users, β_j the coefficient to be determined, k dimension number of polynomial function also chosen by users; $Z(X)$ is a stochastic function, which is considered as a normal distribution $(0, \sigma^2)$ generally.

Let $k=1$ and $f_1(x)=1$, Eq.(1) becomes the ordinary Kriging or DACE (Design and Analysis of Computer Experiment) model^[6-7]:

$$\hat{y}(x) = \hat{\beta} + r(x)^T R^{-1}(Y - \mathbf{1}\hat{\beta}) \quad (2)$$

where $\hat{\beta} = \mathbf{1}^T R^{-1} Y / (\mathbf{1}^T R^{-1} \mathbf{1})$ and $\mathbf{1}$ denote an n -vector of ones. $r(x) = [R(x, x_1) \ R(x, x_2) \ \dots \ R(x, x_n)]^T$, where $R(x, x_i)$ is the correlation between an unknown point and the known sample points.

3. Modified Sequential Kriging Optimization

The SKO method is one of the surrogate model-based optimization approaches, in which the calculation precision is related to the sample points. In order to increase the accuracy of the model in Eq.(2), the expected improvement criterion was introduced in SKO^[7]:

$$\left. \begin{aligned} I &= \max(f_{\min} - Y_d, 0) \\ E[I(x)] &\equiv E(\max(f_{\min} - Y_d, 0)) \end{aligned} \right\} \quad (3)$$

where f_{\min} represents the current best value of the function at known points; Y_d is Normal (\hat{y}, s^2) , in which \hat{y} and s are the output predictor and its square root of the mean squared error (RMSE) respectively. s can be expressed as

$$s^2(x) = \sigma^2 \left\{ 1 - \begin{bmatrix} \mathbf{f}^T(x) & \mathbf{r}^T(x) \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{F}^T \\ \mathbf{F} & \mathbf{R} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{f}(x) \\ \mathbf{r}(x) \end{bmatrix} \right\} \quad (4)$$

where $\mathbf{F} = [f(x_1) \ f(x_2) \ \dots \ f(x_n)]^T = [1 \ 1 \ \dots \ 1]^T$. Then we can get the expected value of the improvement I by calculating the integration as

$$E[I(x)] = (f_{\min} - \hat{y}) \phi\left(\frac{f_{\min} - \hat{y}}{s}\right) + s \varphi\left(\frac{f_{\min} - \hat{y}}{s}\right) \quad (5)$$

where φ and ϕ are the standard normal density and distribution function respectively. Through inserting the maximum EI point as the additional sample point, improvement of the model and robust exploration of the global optimum can be achieved^[8].

3.1. Modified sequential Kriging optimization

Fig.1^[7] gives an example to show how the SKO algorithm works.

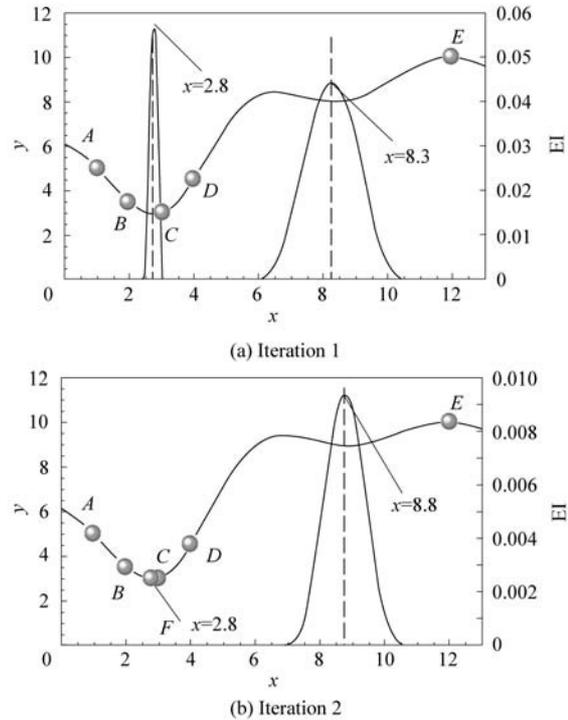


Fig.1 Update Kriging model by EI method^[7].

In Fig.1(a), the curve indicates the Kriging model constructed by 5 points and the line with peaks indicates the EI with two peaks at $x=2.8$ and $x=8.3$. However, the maximum EI is located at $x=8.8$ in next iteration as shown in Fig.1(b), then SKO will add the second sample point there. The conventional SKO algorithm adds the sample point at maximum EI, so SKO algorithm samples the point (point F) at current calculation because the peak at $x=2.8$ is much higher. However, the maximum EI is located at $x=8.8$ in next iteration, then SKO will add the second sample point there. It is obvious that only one point is sampled in each iteration in SKO, so searching the maximum of EI is time consuming, especially in high-dimension problems. In order to solve the above problem, this article presents a modified criterion on SKO through enhancing the number of sample points in each iteration. Now, we use the example shown in Fig.1(a) to describe its motivation.

The main idea of MSKO is to add the points at $x=2.8$ and $x=8.3$ at the same time in the first iteration, viz. we change the twice optimization problem into once, which could decrease the searching times of maximizing EI obviously. Comparing with the SKO that inserts the sample point at $x=2.8$ and $x=8.8$ step by step, the sample points of MSKO are $x=2.8$ and $x=8.3$ in one iteration, so MSKO is faster.

Before re-fitting the Kriging model, the new sample points should be verified according to the following equation:

$$\left\| \mathbf{R}(x_0, x_i) \right\| < 0.001 \left\| \mathbf{R}(x_{LB}, x_{UB}) \right\|, \quad (6)$$

$$i = 1, 2, \dots, n, x_i \in \Omega$$

where x_{LB} and x_{UB} represent the lower bound and upper bound respectively. Eq.(6) can ensure that the new sample points do not overlap the previous one and the distance between two sample points is not too small.

Since EI function values are all positive in the range of $\hat{y} \in [-\infty, f_{\min})$, in which the algorithm can guarantee the new sample point is different from previous one as long as there are unsampled points. Since the number of points is finite, the algorithm will sample all points and the global minimum will be found^[9].

With respect to the termination criterion in Ref.[7], the algorithm will terminate if the expected improvement is less than 1% of the best current function value. Considering the influence of RMSE, it is necessary to keep the RMSE to an acceptable level, so the double stopping criterion is exploited in MSKO as

$$EI_{\max} \leq 0.01f_{\min} \quad \text{and} \quad |y(x^i) - f(x^i)|/s_{x^i} \leq 3 \quad (7)$$

In MSKO we utilize optimization algorithm Divid-

ing RECTangles (DIRECT) to find the maximum EI. The DIRECT is a searching method based on previous collected data without knowing gradient information. Its global convergence property has been proved in Refs.[10]-[11].

3.2. Properties analysis of MSKO

We select a classical mathematic model to describe its properties as

$$z = \frac{1}{1\,000} (4x^2 - 2.1x^4 + \frac{1}{3}x^6 + xy - 4y^2 + 4y^4 + 2\,500 \sin x + 2\,500 \sin y) \quad x, y \in [-5, 5] \quad (8)$$

Ref.[12] gave the optimal solution of this problem: the global minima is $-5.208\,5$ which is located at $(-1.635\,7, -1.153\,8)$ and the local minima are $-2.082\,2$ located at $(3.717\,9, 4.743\,6)$ and $-3.556\,3$ at $(4.230\,6, -1.563\,4)$ shown in Fig.2.

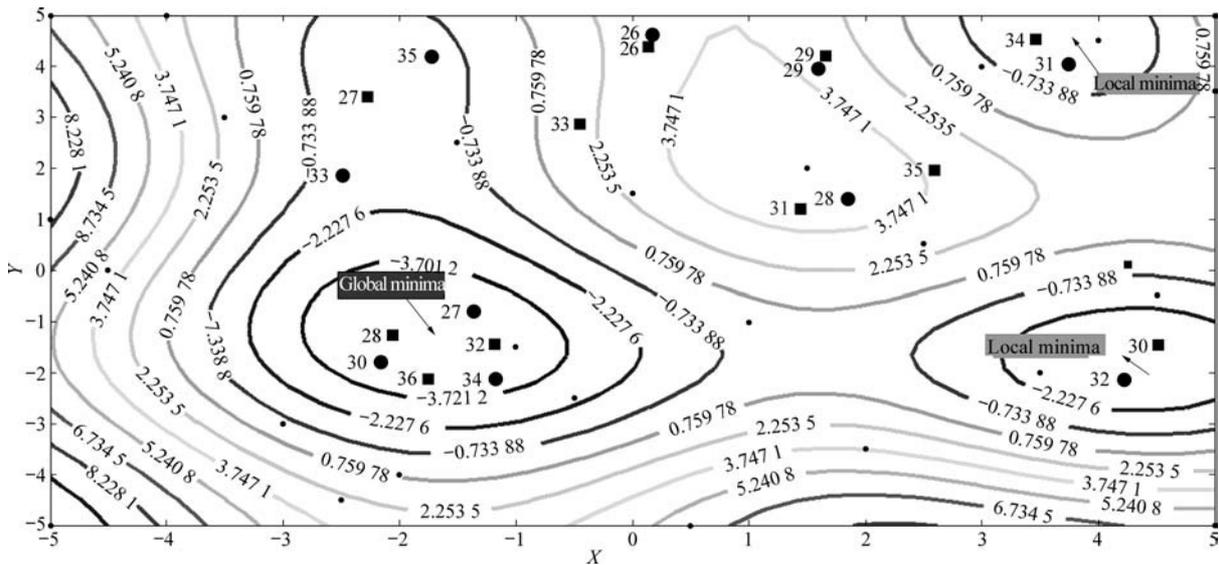


Fig.2 Optimization process and new sample points.

The small dots in Fig.2 represent the initial 25 sample data according to the Latin hypercube strategy while the central textbox is the global optimal solution after optimization. The right two textboxes represent the local optimal solution. The rectangle points and round points indicate the sample points added to the updated Kriging model in MSKO and SKO. The number 26 to 36 near them indicate the sequence of added sample points.

In MSKO, we need 6 iterations, in which the first fifth ones insert 2 points in each iteration and we add one point in last iteration. We can observe the sequence of the added points in MSKO that at first sample points are added in the most uncertain area of the initial Kriging model (upper area) in order to increase the model accuracy. Then the algorithm once finds two

local minima and updates the model but it does not stop there. In the update process, the algorithm calculates the EI according to Eq.(5) gradually to find the larger EI until the convergence condition is satisfied.

On the contrary, the SKO algorithm needs 10 iterations, so the MSKO is faster than SKO even considering the model update.

After giving the computational performance comparison of adding new sample points, now we compare the accuracy between using SKO and MSKO. Fig.3 shows that there is no clear difference in convergence times and optimization value between the two.

In order to verify the global optimization capability of SKO and MSKO, we start the optimization with the initial point $(0,0)$, $(4,3)$ and $(4,-2)$, which are close to

the local minima shown in Table 1.

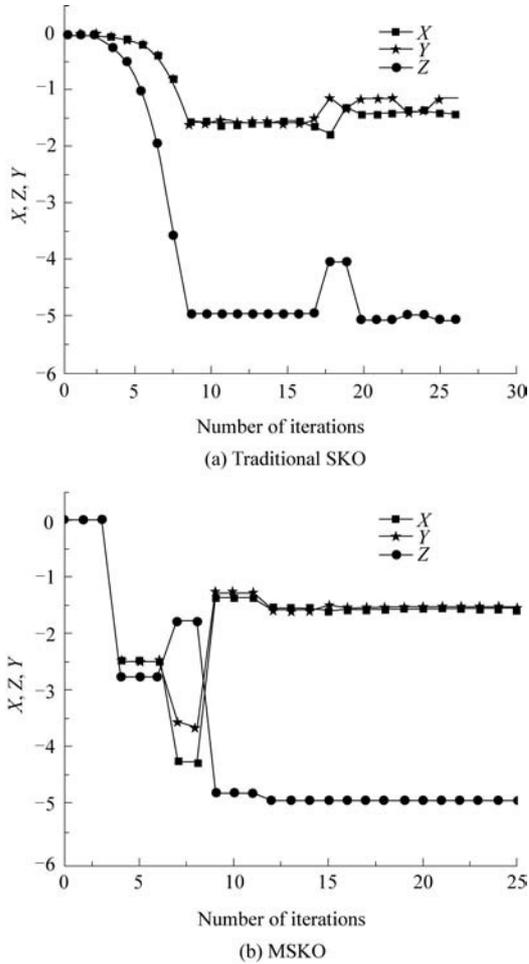


Fig.3 Iterations of SKO and MSKO.

The assessment metrics are selected according to Ref.[5] as follows:

If: The number of iterations required before a point is sampled with an objective function value within $\pm 2\%$ of the true solution.

Ix: The number of iterations required before a point is sampled within a box with the size of $\pm 2\%$ of the design space centered around the true solution.

TN: Total number of iterations when converged.

FS: Final solution of (x, y) .

Dx: The distance from the final solution to the global minima.

RMSE: The global modeling error of final Kriging model.

If, Ix and TN indicate the efficiency of the algorithm; FS and Dx express its accuracy and RMSE denotes the precision of Kriging model. Except FS, the lower the values are, the better the performance is.

From the algorithm accuracy points of view, MSKO can ensure global optimization no matter where the initial point is. From the algorithm rapidity points of

view, the Kriging model can approach the global optimization quickly based on MSKO.

Table 1 Detailed information of SKO and MSKO

Initial point	If	Ix	TN	FS	Dx	RMSE
(0,0)	SKO	7	11	33	(-1.410, -1.154)	0.044 2 0.154 7
	MSKO	3	8	29	(-1.571, -1.542)	0.048 4 0.102 8
(4,3)	SKO	10	7	46	(-1.163, -1.568)	0.155 9 0.298 2
	MSKO	5	11	35	(-1.685, -1.465)	0.002 9 0.206 5
(4,-2)	SKO	11	15	40	(-1.236, -0.641)	0.342 7 0.441 8
	MSKO	5	12	32	(-1.666, -1.465)	0 0.316 2

4. Application to Active Suspension System

We apply the proposed MSKO method to the design of the active suspension system based on electro-hydrostatic actuator (EHA) which originates in aviation field. EHA is an electrically powered actuator incorporating a controlled direction electric motor and hydraulic pump. Active suspension based on EHA has the characteristic of compact structure, large delivered power and being easy to control.

4.1. Active suspension and its subsystem

Active suspension system is a typical mechanical-electrical-hydraulic multidisciplinary complex system. We divide the active suspension system into four subsystems that are mechanics subsystem (Me, rectangle ①), control subsystem (Co, rectangle ②), electronics subsystem (El, rectangle ③) and hydraulic subsystem (Hy, rectangle ④). Fig.4 indicates the relationships and interface among the subsystems. Here, some factors such as tire deflection, damper behavior are neglected.

4.2. Optimization problem modeling

Although there are lots of design variables in real active suspension, we just select the following 8 parameters to model the system for simplicity. We model the optimization problem as follows:

$$\begin{aligned}
 &\text{Find } \mathbf{X}_s = [D \ d \ K_f \ K_a \ l_u \ l_d \ l_k \ l_p] \\
 &\text{min } \sigma\%(D, d, K_f, K_a, l_u, l_d, l_k, l_p) \\
 &\text{s.t. } \Delta l(D, d, K_f, K_a, l_u, l_d, l_k, l_p) \leq 5 \text{ mm} \\
 &\quad T_s(D, d, K_f, K_a, l_u, l_d, l_k, l_p) \leq 0.3 \quad (9)
 \end{aligned}$$

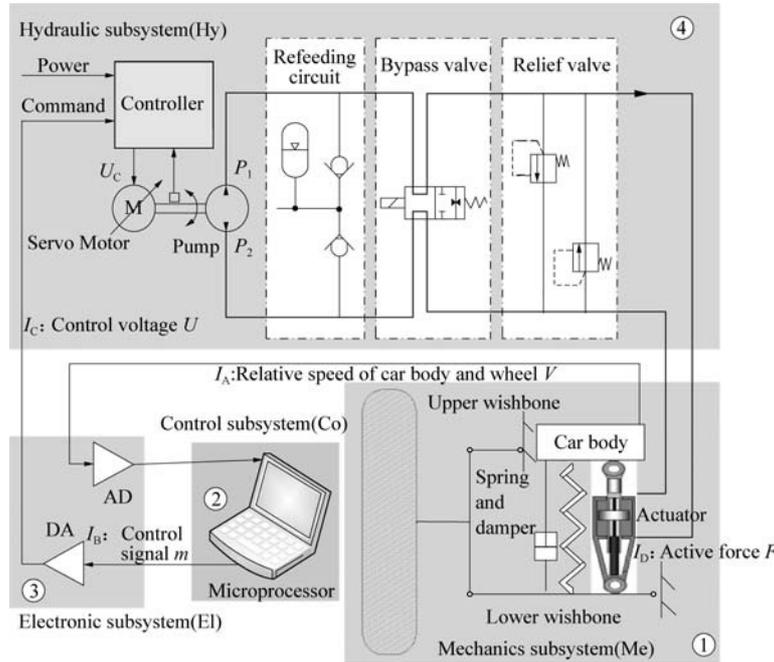


Fig.4 Modeling of active suspension.

where $X_s=[D \ d \ K_f \ K_a \ l_u \ l_d \ l_k \ l_p]$ is design variable, in which D is the external diameter of the piston; d is the internal diameter of the piston, K_a the coefficient of amplifier and K_f the coefficient of displacement sensor. The above four variables are from hydraulic subsystem. And l_u , l_d , l_k and l_p are the length of upper and lower wishbone, kingpin and knuckle which are from mechanical (dynamic) discipline. The parameters K_p , K_i and K_d of fuzzy PID controller from control subsystem are not considered as design vector.

As for the constraining condition, the slip displacement of wheel Δl from mechanical subsystem could not be more than 5 mm viz $\Delta l \leq 5$ mm and the settling time T_s is less than 0.3 s.

The object function is to minimize the overshoot $\sigma\%$ of the vertical displacement of car body. In order to make the optimization problem unconstrained, we merge the constraints into the object function as penalty functions as follows:

$$\begin{aligned} & \text{Find } X_s = [D \ d \ K_f \ K_a \ l_u \ l_d \ l_k \ l_p] \\ & \min \ y(X_s) = (\sigma\%(X_s) + M_1 \cdot \text{Max}(\Delta l(X_s) - 5, 0))^2 + \\ & \quad M_2 \cdot \text{Max}(T_s(X_s) - 0.3, 0)^2 \end{aligned} \quad (10)$$

where M_1 and M_2 are penalty coefficients. With the proposed MSKO method, we can obtain the surrogate model of the system optimization as

$$\begin{aligned} & \text{Find } X_s = [D \ d \ K_f \ K_a \ l_u \ l_d \ l_k \ l_p] \\ & \min \ \hat{y}(X_s) = \hat{\beta} + r(X_s)^T R^{-1}(Y - I\hat{\beta}) \end{aligned} \quad (11)$$

In Eq.(11), $\hat{y}(X_s)$ is updated dynamically during the optimization process according to the augment expected improvement rule.

4.3. Analysis modeling

To calculate Δl , T_s and $\sigma\%$, we need to conduct hydraulic, dynamic and control analysis.

Considering the motor and pump are connected directly, the expression of torque is^[13]

$$T = (J_m + J_p)\dot{\omega} + (K_v + K_f)\omega + T_{DB} + D_p(P_a - P_b) \quad (12)$$

where J_m and J_p are rotary inertia of motor and pump, K_v and K_f viscosity and friction coefficient of motor respectively, T_{DB} is torque loss cause by friction and D_p pump delivery. We can obtain the expression of the angle velocity of pump as^[14]

$$\omega = \frac{CGV_c - D_p(P_a - P_b) - T_{DB}}{(J_p + J_m)s + (K_v + K_f + C_E)CG} \quad (13)$$

where C_E and V_c are motor back electromotive force (EMF) constant and motor input voltage respectively, C and G are torque constant and transfer function separately. The hydraulic pump and actuator equation can be expressed as^[13]

$$D_p\omega = A\dot{x} + \frac{V_o}{2\beta_e}\left(\frac{dP_1}{dt} - \frac{dP_2}{dt}\right) + (\xi + L/2)(P_1 - P_2) + 2\xi P_{pipe} \quad (14)$$

where $A = \pi(D^2 - d^2)/4$ is cylinder force area, β_e oil equivalent volumetric elastic modulus, P_1 and P_2 are entrance and exit chamber pressure of the cylinder respectively, ξ and L are internal and external leak coefficient of pump and P_{pipe} is the pressure drop between pump and cylinder. Then the load force of hydraulic cylinder can be described as

$$F = (P_1 - P_2)A = M\ddot{x} + B\dot{x} + Kx + F_L \quad (15)$$

where F_L represents the external interference force of hydraulic cylinder.

Substitute Eq.(14) by P_1-P_2 and ignore elastic load, then we can get the transfer function of hydraulic component^[14]

$$x = \frac{D_p \omega - 2\xi P_{pipe} - F_L \xi + L/2 \left[\frac{V_0}{2\beta_e(\xi + L/2)} s + 1 \right]}{A \left\{ \frac{V_0 M}{2A^2 \beta_e} s^2 + \left[\frac{V_0 B}{2A^2 \beta_e} + \frac{M(\xi + L/2)}{A^2} \right] s + 1 \right\}} \quad (16)$$

Ref.[15] shows the double wishbone suspension structure. The height of the wheel is h . We need to measure the angle of wheel plane λ and horizontal slip of the wheel Δl .

4.4. Collaborative simulation and optimization

The design software that we choose in our platform includes ADAMS for Me subsystem, MATLAB for Co subsystem and Simulink for Hy subsystem. The integrated design platform is based on Simulink.

With MATLAB, the Simulink simulation model is described in Fig.5. The rectangle part in Fig.5 is the model created by ADAMS, which is exported as the "adams_subsystem"^[16]. The input of the whole system is the height of the ground which is a step function. Through collaborative simulation, we can get the settling time T_s and overshoot $\sigma\%$ from Simulink and horizontal slip Δl from ADAMS.

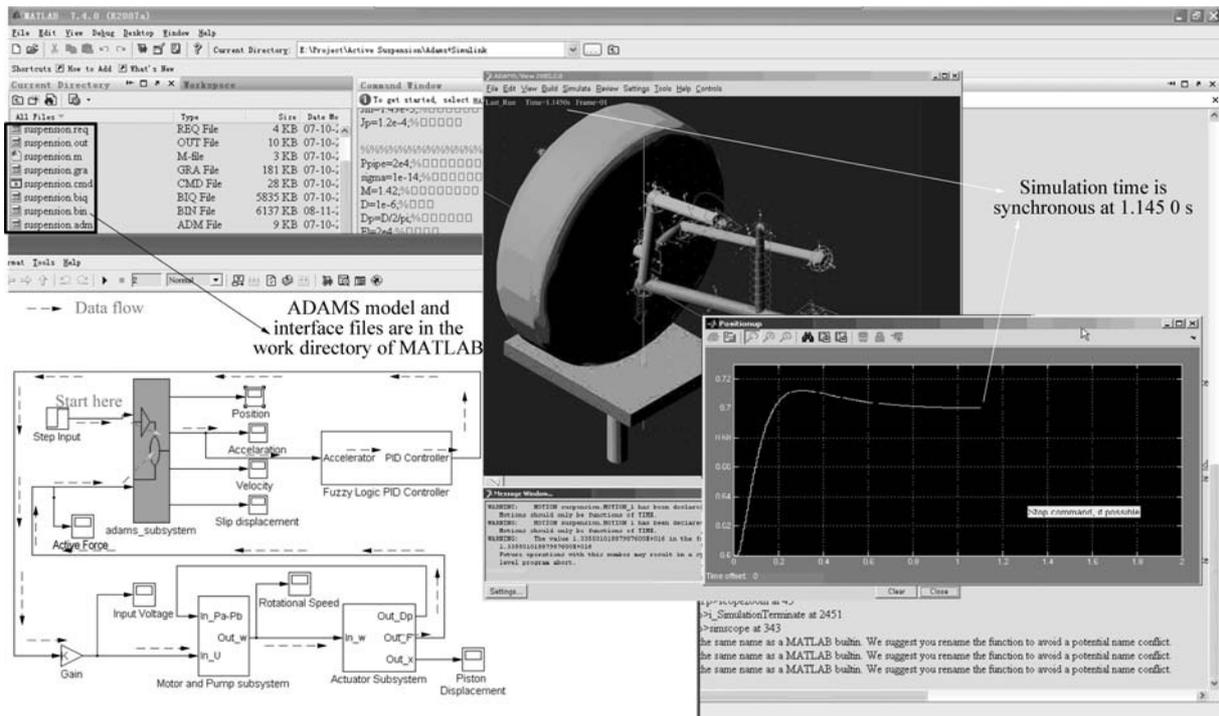


Fig.5 Collaborative simulation of active suspension.

We list the optimization information of the parameters in Table 2, in which the unit is SI except millimeter for Δl .

In Table 2, Para represents the parameter, Ini represents the initial values, LB and UB denote the lower bound and upper bound, Opt and OptS the optimization results of MSKO and SKO; DeV, Cons and ObjF are the design vector, constraint vector and objective function respectively.

If, Ix, TN show the efficiency of SKO and MSKO, and RMSE indicates the accuracy of the final Kriging model. It is obvious that the MSKO converges faster than SKO with small RMSE. Fig.6 shows the iteration process of T_s , Δl and $\sigma\%$.

In Fig.6, the straight lines $y = 5$ and $y = 0.3$ represent the upper bounds of the double constraints respectively. Since the constraint variables are under the up-

per bound finally, the dynamic and control performances of the system are greatly improved.

Table 2 Optimization result of active suspension

	Para	Ini	LB	UB	Opt	OptS
DeV	D	0.20	0.10	0.30	0.142	0.176
	d	0.10	0.01	0.15	0.130	0.124
	K_f	1.10	1.00	1.20	1.025	1.342
	K_a	130	120	150	125.6	119.8
	l_u	0.30	0.26	0.38	0.347	0.356
	l_d	0.48	0.40	0.58	0.390	0.412
	l_k	0.31	0.28	0.40	0.298	0.328
Cons	l_p	0.27	0.20	0.30	0.293	0.275
	T_s	2.12		0.3	0.26	0.29
	Δl	12.5		5	1.8	1.97
ObjF	$\sigma\%$	8.57			1.43	1.69
		If	Ix	TN	RMSE	
	SKO	8	25	32	0.544	8
	MSKO	12	16	26	0.343	1

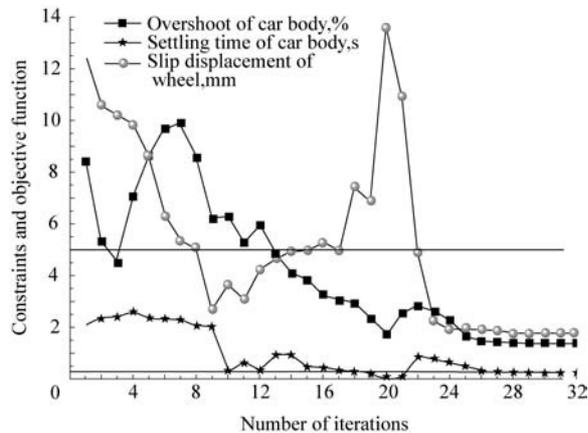


Fig.6 Iteration of constraints and objective function.

5. Conclusions

The contribution of this article is to use surrogate model-based global optimization method to deal with the complex product optimization problems which involve multiple computer simulation tools. The detailed contributions are summarized as follows:

(1) The drawback of EI function in SKO is time consuming due to that one new point is inserted at the maximum EI in one iteration. This article proposes the MSKO algorithm, in which we change the twice optimization problem into once through adding more than one point at the same time.

(2) Before re-fitting the Kriging model, the new sample points are verified to ensure that they do not overlap the previous one and the distance between two sample points is not too small.

(3) This article presents the double stopping criterion to keep the RMSE of the final surrogate model at an acceptable level. When the algorithm converges, the Kriging model is accurate enough.

Application of active suspension system optimization indicates that MSKO could improve the convergence speed under small RMSE, so it is suitable to the engineering problem based on collaborative simulation.

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