Parameter Turning of PID Controller Based on Molecular Beacon DNA Computing

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***Abstract*—Molecular beacon deoxyribonucleic acid computing is new research focus of intelligent control theory in recent years, it is also new bionic algorithm. It is well known that a very important problem how to determine or tune the proportional integral derivative controller parameters, because these parameters have a great influence on the stability and the performance of the control system. Parameter turning of proportional integral derivative controller by using molecular beacon deoxyribonucleic acid computing can avoid system early-ripe and find global optimal solution rapidly. Molecular beacon is a single strand of deoxyribonucleic acid base pairs formed their own part of the hairpin-like fluorescent probes, the use of molecular beacon can readily detect the concentration of deoxyribonucleic acid molecule which matching with it in test tube, the result of detection can decide which need to be copied and which need to be discarded. The molecular beacon deoxyribonucleic acid computing has high reliability and easy operation for proportional integral derivative controller parameter tuning. The result of simulation proves that molecular beacon deoxyribonucleic acid computing algorithm has distinct advantages than traditional algorithm. molecular beacon deoxyribonucleic acid computing is bound to has very great impact on intelligent control in the future.**

***Index Terms*—Deoxyribonucleic acid computing, Molecular beacon, PID controller, base pairing, parameter tuning**

I. INTRODUCTION

Proportional Integral Derivative (PID) controllers are the most adopted controllers for industrial plants, mainly because, despite their simplicity, they can assure satisfactory performances for a wide range of process control system. Therefore, the cost/benefit ratio they provide is difficult to achieve by other controllers. To simplify the operators work, many tuning formulas which are for to determine PID controller parameters have been devised in the last 60 years. Three parameters which are proportional gain, derivative time and integral time of the PID controller must be determined and tuned to obtain a satisfactory closed-loop performance. Methods to tune the parameters of PID controllers are very important for the process industries. In recent years, deoxyribonucleic acid(DNA) computing has been documented in various literatures Since Adleman's solution to the Hamiltonian Path problem [1], DNA and RNA solutions of some other famous NP-complete problems, such as the maximal clique problem, the 3-SAT problem and the knight problem, have been given. Some important progresses have been made in the technologies in computing with biomolecules. DNA computing takes DNA molecular as vector, makes biochemical reaction, when stimulated by enzyme and optimum temperature, and gets optimal solution finally. This model has advantages, which can't be replaced by other algorithms, such as huge parallelism, fast operation, great information storage, lower energy dissipation, abundant resources, and simple operation, and especially for certain autonomy of the synthesized DNA molecular. In 1996, Ogihara put forward the simulation of boolean circuit based on DNA, and gave the implementation method of DNA logic circuit [2]. It has epoch-making significance for design of DNA chip in future. By exploration and research for more than ten years, DNA computing has achieved great progress, not only on theoretical research, but also on hardware circuit. It declares the coming of bio-computer era, along with the DNA-computer is published. In this paper, we propose a new tuning method of PID parameters included in the tuning PID parameters proposed previously are sought using molecular beacon DNA computing. This paper is organized as follows. Section 2 the DNA encoding mechanism is introduced. Section 3, working principle and application of molecular beacon is presented. Section 4, PID controller based on DNA molecular beacon is designed. Finally, Section 5, experimental results and discussed.

II. MECHANISM OF DNA ENCODING

DNA is short for Deoxyribonucleic acid, and is a biomacromolecule, composed by four nucleotides, which are adenine (A for short), cytosine (C for short), guanine (G for short), and thymine (T for short). And each nucleotide consists of a phosphoric acid group, pentose and nitrogenous base (adenine, cytosine, guanine and thymine). On the basis of principles of Watson-Crick base pairing (namely, A-T, C-G), two deoxyribonucleotide chains forms double helix structure,

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which is DNA molecules. If put it into a test tube, and also with corresponding enzyme and adaptive temperature, DNA molecules will be cloned spontaneously, and maybe, gene will recombine and mutate, which forms daughter DNA with biodiversity. Form Darwinian evolution, the final outcome of evolution is survival of the fittest, so, All that's left is the one with best adaptability. On this, researcher thinks of, if making our problem, which needs to be solved, encoded to DNA chains by an encoding mechanism, so, it can find the optimal solution by itself biochemical reaction. This method has high reliability, simple operation, large processing data and fast computing speed. Then, it discusses how to encode for a practical problem.

The encoded mode is flexible. It can select different methods for practical problems. First, encoding mechanism using binary: from biology, in double helix structure of the DNA molecule, it is double hydrogen bonding when A and T make base pairing, and we take this as 0 (or 1); it is three hydrogen bonding when C and G make base pairing, and we take this as 1 (or 0). For converting practical problems to DNA chains, it achieves by binary code mechanism of DNA. And then, after a series of biochemical reaction, it gives the best DNA chain. Last, it can get the final optimal solution by decoding, which also is the one we need. For example, the base pairing on DNA chain is: AGGTTCAACGTTT…, so the corresponding binary string is: 0110010011000…. If the marshalling sequence of bases is different, the binary string is different too. Namely, if there are n bases, it can have 2^n binary strings [3]. Thus it can be seen, it has great ability for DNA chain to store information. In addition, quanternary coding is also frequently-used. It takes T as 0, C as 1, G as 2, and A as 3. Their corresponding binary are: T=00, C =01, G=10, A=11. For a DNA chain with AGGTTCAACGTTT…, its corresponding binary string by quaternary coding is: 11101000000111110110000000…. So, if there are n bases, it can have 4^n binary strings. It has higher utilization than binary coding. So, it mainly use quaternary coding in this paper. If define a digraph G=(V, E), its vertices V={$\upsilon_s, \upsilon_0^0, \upsilon_0^1, \upsilon_1^0, \upsilon_1^1 \cdots \upsilon_n^0, \upsilon_n^1$}, which υ_s is initial vertex, υ_j^i(i=0,1; j=0,1…n) expresses the j-th from right of binary string. Set of edges is E={$\upsilon_s \upsilon_0^0$, $\upsilon_s \upsilon_0^1$, $\upsilon_0^0 \upsilon_1^0 \cdots \upsilon_{n-1}^1 \upsilon_n^0$, $\upsilon_{n-1}^1 \upsilon_n^1$}. The digraph is showed in Fig.1 [4].

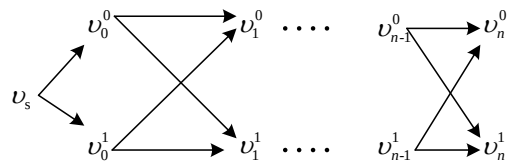

Figure 1. The vector digraph of binary strings.

From Fig.1, each edge is a base when using quaternary coding. For a practical problem, coding can be realized by bases directly or by this digraph. And two methods can make simultaneously, which has high speed and reliability. Each route in digraph, passes each node at least once, called a Hamilton path.

III. MECHANISM OF MOLECULAR BEACON

Molecular beacon is stem ring double marking oligonucleotide probe, which is hairpin structure formed by part of bases complementation in single-stranded DNA. Generally speaking, inner ring of molecular beacon has 15~30 bases, and it can make pairing with target molecules which need concentration detection; there are 5~8 pairs complementary bases in stem area, and its tail end is the 5’ and 3’ end, which are used to connect fluorescent group and quenching group respectively.

The frequently-used fluorescent and quenching group are: coumarin (blue)-dimethyl amino nitrogen benzoyl accidentally (DABCYL), EADNS (blue-green)-DABCYL, fluorescein (green)- DABCYL, Lucifer yellow (yellow)- DABCYL, Texas Red-DABCYL [5], whose structure chart shows in Fig.2 [6]. Under annealing temperature and because of hairpin structure, fluorescent and quenching group are huddled together, and photons which generated by fluorescent group are quenched by quencher, so we can’t see them. When heating molecular beacon, and making them pairing with target molecules in liquid (the DNA template pairing with bases of inner ring of molecular beacon), the loops of molecular beacon are opened, and the corresponding fluorescent and quenching group are separated. The quenches role is relieved, so we can see the fluorescence when fluorescence group is aroused and generates photons. Because of the existence of enzyme cutting effect, molecular beacon can accumulate fluorescence, so the brightness of corresponding molecular beacon will be strong, if concentration of target molecules is higher. Based on this, it can make living analysis, clinical diagnosis and genetic testing.

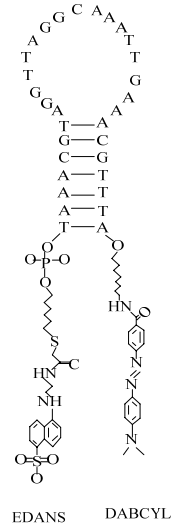

Figure.2 The basic structure of molecular beacon

Now, the types of molecular beacon which has been proposed are: single fluorescence groups molecular beacon, lock molecular beacon, acaulescence molecular beacon, fluorescence wavelength transfer molecular

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beacon. According to different experimental requirements, select different molecular beacon to test. Along with the deepening of the research, molecular beacon has developed, from DNA to PNA and then to LNA. Application fields are also broadened, from timed and quantitative analysis of PCR product, analysis and development of allele, analysis of DNA base mispairing to metabolism analysis of nucleic acid of living body, and analysis of interaction between DNA and protein. In general, molecular beacon has become the essential tool of bioscience gradually.

The combined ability between molecular beacon and target molecule is different, and it takes Signal to background ratio as measurement criteria of cross performance [8]:

$$SBR = (F_{hybrid} - F_{buffer})/(F_w - F_{buffer}) \quad (1)$$

Which, F_{hybrid} is fluorescence intensity after pairing between selected molecular beacon and target molecule; F_{buffer} is fluorescence intensity of buffer solution in test tube; F_w is fluorescence intensity of selected molecular beacon. If the type of selected molecular beacon is different, these values are different too.

The working principle of molecular beacon shows in Fig.3:

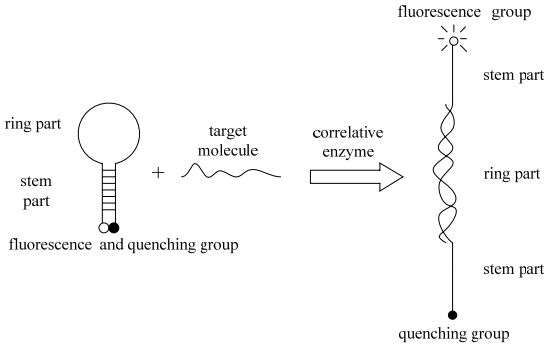

Figure.3 The working principle of molecular beacon

From Fig3, when fluorescent probe which is hairpin structure, encounters target molecule (single-stranded DNA), and under correlative enzyme, its ring part will make pairing with target molecule according to watson-crick base complementation pairing rule. The hairpin structure opens and then become the reverse double helix structure. And now, fluorescence and quenching group are separate, and then fluorescence group give out light and accumulate fluorescence. If concentration of target molecule is higher, the brightness of probe will be higher too. It reaches the goal of selection.

IV. PARAMETER TUNING OF PID CONTROLLER BASED ON MOLECULAR BEACON DNA COMPUTING

PID controller is used broadest in industry, and has mature technology. And now, it also has many improved types, such as robustness PID controller, PI controller, PD controller. But fractional order PID controller is the inevitable trend in future. The selecting of three parameters is important for PID controller. The effects of PID controllers with different parameters is great different. PID parameters turning is first proposed by Ziegler and Nichol in 1942, which aims to first order inertia and pure delay, called Z-N method [7]. Now, there have many methods to adjust PID parameters, such as fuzzy control, neural network and genetic algorithm. But, these algorithms all have some problems, such as slow convergence rate, falling into the local optimal solution. DNA algorithm solves them, and the concrete operating process resumes as follows:

The three parameters of PID controller are k_p, k_i and k_d. Which, $k_p \in [0, m]$, k_i, $k_d \in [0, n]$. The law of PID controller is: $u(t) = k_p error(t) + k_i \int_0^t error(t)dt + k_d \frac{derror(t)}{dt}$, which, $u(t)$ is output of controller. $error(t) = rin(t) - yout(t)$, which, $rin(t)$ is the real input. First, make binary coding for three parameters, and it can be realized by MATLAB:

```
Minkp=zeros(1);
Maxkp=m*ones(1);
Minki=zeros(1);
Maxki=n*ones(1);
Minkd=zeros(1);
Maxkd=n*ones(1);
E=round(rand(size,3*Codel));
Kp=E(j,1:Codel);
Ki=E(j,Codel+1:2*Codel);
Kd=E(j,2*Codel+1:3*Codel);
```

Which, size is the size of selected training sample, namely, population size (individual in population, namely, candidate solution of the practical problem); j expresses the j-th individual; Codel expresses the binary digits of each parameter. Thus, the problem become selecting the best individual from population, in which the parameters can get the desired output. How to find the best individual? From Darwin's theory of evolution, the individual is left, which has best fitness to environment. And this fitness function (target function) is the constraint condition of practical problem. So, it is to select the individual which has the largest fitness function value. Using the converting from binary string to DNA chain, introduced in the second part, the best individual in Fig1, is the shortest path problem, from initial point to terminal point, and also is the postman path problem.

The follow contents introduce that the DNA molecule which represents candidate solutions how to proceed biochemical reaction to find the DNA molecule which represent optimal solution. First of all, randomly generated the candidate group which size is N, set the evolutionary number of maximum as G(this article set G is 100). Step1: Encode the candidate solution of actual problem by using DNA coding principle, now the candidate solution become many single DNA molecules and take the DNA molecules which are complementary with every single as molecular beacon probes.

Step2: Calculate the fit values of every DNA molecule, select two parent DNA molecules by using the principle

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that the bigger fit values the bigger possibility of choice and put them into tubes, add the exonuclease, restriction enzymes and DNA ligase into test tubes, set the temperature of test tubes as 55° , enzyme activity can completely come into play in this temperature, offspring DNA molecules take parent DNA molecule as a template proceed recombinant, replication and gene mutation.

Step3: Construct Molecular beacon probe of offspring DNA molecules for detecting its concentration, the new descendants DNA mixed with the original DNA become the same scale population that is elitism.

Step4: Pick out the individual of which the maximum by using molecular beacon detecting, the rest of DNA molecules in test tube continue act, after proceeded a number of reactions if there are not individual whose fit value is better than the individual's whose concentration is biggest then the biochemical reaction to end, if the individual can be found that is to say the former reaction fall into local optimal value. Repeat step 2 to step 4, there use of disastrous ideological can guarantees algorithm's efficiency and reliability.

Step5: When find the individual whose fit value is the best or the end condition were met, the reaction end.

In step 2, the role of adding exonuclease is hydrolyze the nucleotide of nucleic acid chain; The role of adding restriction enzymes is identifying nucleotide sequences and cutting DNA from fixed position inside DNA molecules; The role of adding DNA ligase is connecting the DNA pieces together into a long DNA molecule. Enzyme equivalent of catalyst in chemical reactions, The reaction formula is:

$$E + S \underset{k_{-1}}{\overset{k_1}{\Leftrightarrow}} ES \overset{k_2}{\Rightarrow} E + P \qquad (2)$$

Where E is the enzyme, S is the catalytic substrates, ES is the complex of enzyme and substrate, P is the products, in the action process, the mass of enzyme will not change. The optimal solution is the shortest path from the initial point to terminal (that is the shortest generalized Euler's track) in figure 1, when the path is shortest the length of corresponding DNA molecule will be the shortest, so there are two methods are used to pick up these DNA molecule:

The first method is: Put the mixture of the tube on the affinity chromatography column, the chromatography column can combine specific molecular substance (such as polymers or hydrophobic silica), those single molecule which have affinity to the chromatography column will be captured. These molecules can be eluted by using eluent, through strictly graded elution we can collect different DNA molecules that is those DNA molecules which have different affinity. This method has very strict requirements to the salt concentration of the eluent, because when the salt concentration of the eluent is different we will get different DNA molecules.

The second method is Agarose gel electrophoresis method: By using molecular sieve effect of agarose gel, those macromolecules will be filtered out for the resistance when they are moving. Agarose gel distinguishable can distinguish these DNA fragment of which difference are 100bp. The separation range of agarose gel separation range is 0.2-20kb, when use Pulsed electrophoresi the separation range can reach up to 10^7bp, use this method we can obtain the shortest DNA molecules.

V. EXAMPLE OF SIMULATION

Take $G(s) = \dfrac{400}{s^2 + 50s}$ as the object of study, input signal $rin(t)$ is step signal，and make kp $\in$[0,20], ki, kd $\in$ [0,1]， establish objective function by using ITAE method:

$$J = \int_0^\infty (\omega_1 \mid e(t) \mid + \omega_2 u^2(t) + \omega_4 \mid ey(t) \mid) dt + \omega_3 \cdot t_u \ ,$$

where $\omega_4 >> \omega_1$, ω_1 =0.999, ω_2 =0.001, ω_3 =2.0, ω_4 =100, $ey(t) = yout(t) - yout(t-1)$, $yout(t)$ is output of system. For convenience we take the reciprocal of objective function as fitness function, when the individual has optimal fitness in fact it has the minimum value of objective function, the block diagram of whole system was shown as follows:

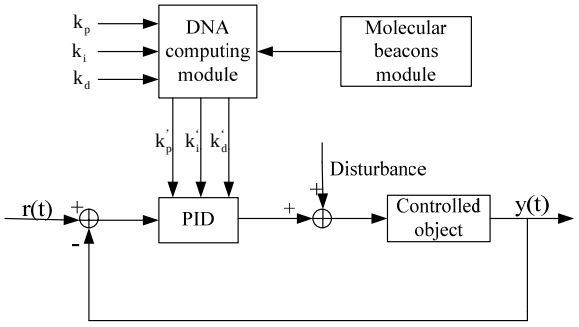

Figure.4 The block diagram of system

The situation of every generations' reactions were shown in the following table:

TABLE I.
THE SITUATION OF EVERY GENERATION'S OPTIMIZING IN BIOCHEMICAL REACTION

The number of iterations	Optimizing			
	DNA encoding	kp	ki	kd
1	AATTCGAGCTAATTT	2.3069	0.1183	0.6999
2	CACGATCTATTTTTT	10.3030	0.1535	0.0147
3	TTTTATCTATTTTTT	17.1652	0.1955	0
4	TCATAAATATTTTTT	15.0147	0.1955	0
5	CGCAAGTCTGTTTTT	16.1095	0.2023	0
. . .	. . .	. . .	. . .	. . .
20	CGCAAAGCATTTTTT	19.5112	0.2258	0
21	CGCAAAGCATTTTTT	19.5112	0.2258	0
22	CGCAAAGCATTTTTT	19.5112	0.2258	0
. . .	. . .	. . .	. . .	. . .
100	CGCAAAGCATTTTTT	19.5112	0.2258	0

As can be seen from table, the speed of optimizing is

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very fast, only through 20 times the DNA computing module found the optimal solution.

Compare these control effects that based on genetic algorithm, fuzzy control algorithm, BP algorithm of neural network and DNA algorithm, the compared results as shown in Fig. 5.

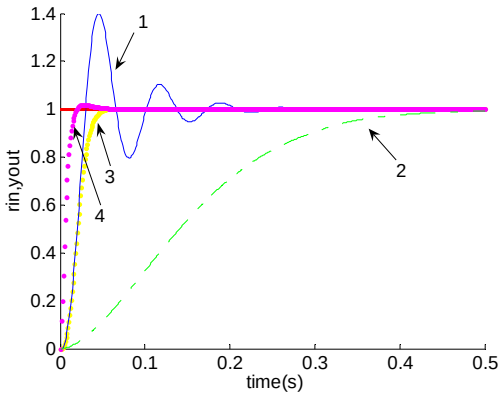

Figure.5 Comparison of different output under different algorithm

The curve 1 is output of the PID control system based on fuzzy control algorithm, the system has vershoot and oscillation, this is mainly because in fuzzy control rules were selected exclusively rely on researchers' experience, once selected improperly, the output is not ideal and the whole system has the defects such as not has learning ability; The Curve 2 is output of PID control system based on genetic algorithm, although there was not overshoot and oscillation output, the rise time is very long, in industrial production this need to avoid. Genetic algorithm has the defects that it is easy fall into local optimum; The curve 3 is the output of the PID control system based on BP neural network, Although control effect is better than curves 1 and 2, rise time not is very ideal and BP algorithm has many defects, for example BP algorithm is very sensitive to initial weight; Although use gradient descent method for training it often stayed on flat region of gradient curved surface; BP algorithm is prone to overtraining; there is no complete theory to determine the number of hidden layer nodes of networks;The curve 4 is the output of the PID control system based on DNA algorithm, Whether in rise time or robust DNA algorithm is significantly better than other algorithms and the operation is easy, The whole optimization process is spontaneous ongoing under the action of DNA molecule. The speed of optimizing is very fast and the algorithm has high reliability. DNA algorithm as a new kind of Bionic algorithm is gradually studied by more and more people.

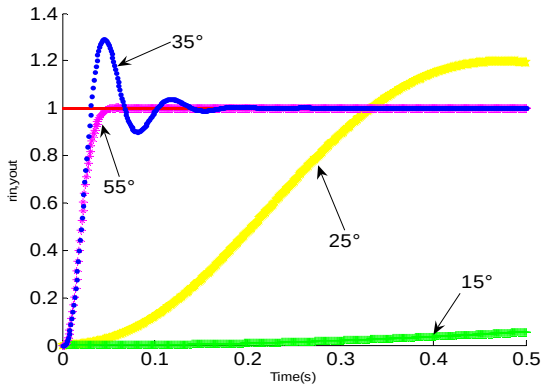

Figure.6 Effects of different temperatures on the experimental results

The key steps of DNA algorithm is under the action of the enzyme DNA molecules' copy and clones, We know that at a temperature of 37 ° enzyme's activity is the most powerful, in this temperature the number of DNA molecules' recombinant and replicated is the largest. There give different curves of DNA Molecular biochemical reactions under different temperatures, it is shown in Fig. 6.

As can be seen from the figure the temperature has large effect on output, if the temperature is inaptitude the solution not is the global value, the output curve will take on large overshoot, frequent oscillation. In figure 6 as the temperature increase the control effect become better and better, rise time become shorter and shorter, the mainly reason is that the more higher temperature the stronger enzyme activity. But when But when the temperature exceeds a certain point the enzyme will denature, corresponding biochemical reaction stop and whole optimize process stop, so keep in mind that the experiment are carried out must at the right temperature.

VI. CONCLUSIONS

DNA computing has been researched by more and more researchers, at present DNA sensor and DNA chip has been introduced, it proclaimed the coming of biological molecules' era. To traditional methods DNA algorithm is reliable, simple and fast, it can process a large group, General algorithm is very prone to instability and paralysis for very large groups, but DNA algorithm can handle huge amounts of data due to the characteristics of its own coding and it has high degree of parallelism in carrying out biochemical reactions, These two features make up for the fatal defects of traditional computers. This article also describes a molecular fluorescent probe—molecular beacon, due to its low background signal, high sensitivity, strong specificity and homogeneous phase detection, it has achieved rapid development in just a few years. Now new patterns molecular beacon have solved the defect that molecular beacon is prone to appear false-positive signals. With the development of gene chips and microarrays, Molecular beacons not only be applied in the tube solution but also be applied in the substrate surface. The synthesize of DNA algorithm and molecular beacons present a new and

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efficient method for the setting of PID controller, control theory is bound to occur a great leap from programming languages to biological science experiment.

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