A novel approach to complex problems has been previously applied to graph classification and the graph equivalence problem. Here we consider its applications to a wide set of NP complete problems, namely, those of finding a subgraph $g$ inside a graph $G$.

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I. INTRODUCTION

In many areas of physics, biology, economics and other fields we encounter “Complex Problems”. Such problems, like finding ground states in spin glasses\(^1\) (or “frustrated” systems in general), folding proteins once the sequence of amino acids is known, or “The Traveling Salesman” problem\(^2\) (and the closely related “Hamiltonian Path” problem for graphs) may appear to be very different. Yet the complexity of these and a host of other problems stems from a common source: There are many, often conflicting, requirements on the elements that embody the solution.

An archetypical\(^2\) example is the “Satisfiability Problem”,\(^3\) where \(O(n)\) requirements are imposed on \(n\) elements. We are asked if all can be simultaneously satisfied, and if so, to actually exhibit the solution. The difficulty in trying to piece out a solution is that we need to make discrete, binary (yes or no) decisions at each step. We are guided by the underlying constraints and/or the desire to minimize the overall “energy” or “cost”. Yet due to the frustrations/conflicts there is no clear strategy for making such choices so as to consistently move towards the solution. “Improvements” obtained at some stage may be later undone and particular choices may exclude other choices many steps later.

Thus if certain pairs of amino acids are near each other in a tentative folded protein, then the demands imposed by the primary sequence and/or excluded volume prevent us from bringing certain other pairs into close proximity. Also visiting a certain vertex excludes, by the very definition of the Hamiltonian path, its future use in trying to complete our tour of the graph.

We suggest a novel approach for addressing such problems:

(i) Instead of performing discrete, maximal, changes of just two elements at a time, we perform at each stage small changes of all elements.

(ii) The original system is mapped onto a simple “physical” model with \(n\) degrees of freedom. To have maximal symmetry so as to avoid biasing in the initial state, and in order to minimize/exclude frustrations, the model is embedded in \(d \approx n\) dimensions.

(iii) We endow our model with a first-order, deterministic dynamics and (numerically) evolve it for some time. The “dynamics”, i.e, the forces between the various elements, is chosen in such a way that if a solution exists, then the initial model evolves into a
specific final form from which the solution is readily inferred.

Ideally we will be able to show that this can be achieved in a polynomial number of steps.

The above are general principles. For each problem we need to specify the model, its
dynamics and prove/verify that it indeed achieves the solution (hopefully in polynomial
time). To date the above approach has been applied to two problems in graph/network
theory:

First [GJN][4] used a symmetric $n$ simplex model in $n$ dimensions. Its evolution identifies
in polynomial number of steps via geometrical bunching of sets of points, various “clusters”
or “Imperfect Cliques” in the graph and assesses the “Communication Distance” between
them (Clusters are groups of vertices with higher than average mutual connectivity.)

Second [GN][5] have shown that the same algorithm solves, in even a shorter time, the
graph equivalence problem (GEP) which is defined as follows: A non-directed graph $G$
with $n$ vertices is specified by a connectivity matrix $C(i,j)$ with entries 1 (or 0) if vertices $i$ and
$j$ are (not) connected. We are given two such connectivity matrices $C$ and $C'$. Are these
matrices representing the same graph and, in the case that they do, can we exhibit the
permutation which makes them identical?

The first problem of approximate graph characterization (AGC) has considerable practical
importance as many networks are likely to have “Hidden Clusters”. Also the GEP was not
solved to date in polynomial time.

Can our novel approach be applied to the NP complete problems?[2] The difficulty of
these problems could manifest—albeit in rather subtle ways which are of interest in their
own right—also in the present approach, preventing a solution in a polynomial time. Thus
for any physical model and any dynamics that we invent in our effort to solve an NP complete
problem, an extremely long time, say, $t = exp(a.n)$, could be required in order to converge
to the solution.

This would be the case if dynamical models emulating any NP complete problem
necessarily have chaotic unstable motion. Alternatively the true minimum energy state of the
system—which is the desired solution—could be masked by a plethora of local minima in which
our system will be trapped almost indefinitely. We cannot exclude the above possibilities.

Still we conjecture that our novel approach is applicable to NPC problems. We are
presently attempting to prove this by actual implementation of this new approach in specific
codes.
All the problems of finding a specific sub-graph $g$ (with $n$ vertices) within a graph $G$ (with $N$ vertices) are NPC. These include finding the largest perfect clique and finding a Hamiltonian circuit. These problems can be reformulated in our approach as searching a perfect dynamically generated “Docking” of a physical model of $g$ onto some subset of vertices/edges of $G$. This is discussed in Sec. III, utilizing evolution in $(N + n)$ dimensions.

II. BRIEF REVIEW OF PREVIOUS APPLICATIONS

To introduce notation and illustrate the ideas, we briefly review earlier applications to the AGC[4] and GEP[5] problems. Consider a symmetric $n$ simplex in $(n - 1)$ dimensions whose vertices $\vec{r}(i)$, represent the abstract vertices $V(i)$ of the graph.[6] We introduce attractive (repulsive) interactions between the points $\vec{r}(i)$ and $\vec{r}(j)$ if the corresponding vertices are (or are not) connected in the original graph:

$$U = \sum_{i>j} U_a(|\vec{r}_i - \vec{r}_j|)C_{ij} + \sum_{i>j} U_r(|\vec{r}_i - \vec{r}_j|)(1 - C_{ij})$$  \hspace{1cm} (1)

The $n$ points then move under the resulting forces:

$$\mu \frac{d\vec{r}_i(t)}{dt} = \vec{F}_i(\vec{r}_i(t))$$ \hspace{1cm} (2)

according to

$$\vec{F}_i = -\nabla U(\vec{r}_i)\{U [\vec{r}_i, \cdots, \vec{r}_n]\}$$ \hspace{1cm} (3)

The first order dynamics ensures that the system consistently moves in the fastest way towards its minimum without the “overshoots” and oscillations of the second-order formulation. In $(n - 1)$ dimensions all the distances $|\vec{r}(i) - \vec{r}(j)|$ are independent (apart from constraints due to triangular inequalities). A monotonic $u(r)$ then excludes any local maxima, minima or saddle points. Thus the system cannot be trapped in any local minimum and will attain its absolute minimum at a boundary point.

After a sufficiently long evolution the original symmetric simplex will be significantly distorted in a way which reflects the topology of the graph in question. Specifically, points $\vec{r}(i)$ representing vertices $V(i)$ which are “close in the graph”, i.e., have many short paths connecting them in the graph, tend to move closer in space. Conversely, points which are “far in the graph”, i.e., have only longer connecting paths tend to move apart.
The original set of $n(n - 1)/2$ $C(i, j)$’s then gets mapped onto the $n(n - 1)/2$ distances $|\vec{r}(i)[t] - \vec{r}(j)[t]| = R(i, j)$. An identical evolution of an equivalent (permuted) $C'(i, j)$ yields another “distance-matrix”, $R'(i, j)$. $R'$ is obtained from $R$ via the same similarity permutation which maps $C$ into $C'$. In general the elements of $R$ (or $R'$) are—unlike those of $C$ and $C'$—all different. Verifying that $R$ and $R'$ are obtained by vertex re-labeling, and finding the required permutation can then be easily done in $O(n)$ steps.

The dynamical evolution above is simulated by using:

$$\vec{r}_i(t + \delta) = \vec{r}_i(t) + \frac{\delta}{\mu} \vec{F}_i(\vec{r}_e(t))$$

Altogether there are $n \cdot v$ edges in the graph with $v$ the average valency (the valency is the number of edges impinging at a vertex). In each simulation step we compute $n \cdot v$ forces $F(i, j)$. Since each force has $(n - 1)$ components we need altogether $O(n^2 \cdot v)$ computations per step. The “size” of the problem $n$ is thus (polynomially) reflected in the number of computations in each step. Note, however, that since in each iteration step all the points move, the number of iteration steps, $s$, required for graph comparison, and/or clustering, need not grow at all with $n$. In many cases the valency $v$ is also $n$ independent and the complexity of the algorithm is only $O(n)$!

III. APPLYING THE NOVEL APPROACH TO NP COMPLETE PROBLEMS

So far we utilized motions of the $N$ points of an $N$ simplex in $N - 1$ dimensions to model problems associated with one graph $G$ with $N$ vertices. Also to test if $G$ and $G'$ are equivalent we separately processed the corresponding simplexes $S$ and $S'$.

For the task of finding a replica of a “small” graph $g$ with $n$ vertices inside a “big” graph $G$, we introduce one extra $(n - 1)$ dimensional $n$ simplex $s$, corresponding to $g$. To better emulate certain complex problems we may allow $S$ and $s$ to be non-symmetric and non-rigid. For now we keep both $S$ and $s$ rigid, symmetric and with a common edge length:

$$|\vec{R}(I) - \vec{R}(J)| = a = |\vec{r}(i) - \vec{r}(j)| \quad I \neq J = 1...N; i \neq j = 1...n$$

Let $C(I, J)$ and $c(i, j)$ be the connectivity matrices for $G$ and $g$, respectively. The small graph $g$ can be found inside $G$ if, and only if, a combinatorial perfect docking of $s$ inside $S$ is possible. The latter is defined as follows:
All edges of \( g \) represented in \( s \) by \( \vec{r}(i) - \vec{r}(j) \) with \( c(i, j) = 1 \), match edges in \( G \) represented in \( S \) by \( \vec{R}(I) - \vec{R}(J) \) with \( C(I, J) = 1 \). Likewise missing edges in \( g \) should also correspond to missing edges in \( G \). In our model it means that the representative vectors in \( s \), namely, \( \vec{r}(i) - \vec{r}(j) \) with \( c(i, j) = 0 \) should dock onto \( \vec{R}(I) - \vec{R}(J) \) with \( C(I, J) = 0 \).

Our choice of symmetric, equal edge simplexes \( S \) and \( s \) allows a geometric match of \( s \) with any symmetric \( n \)-sub-simplex; i.e., any \((n-1)\) dimensional “Face” of the large simplex \( S \). We next introduce interactions between the edges of \( s \) and those of \( S \) which correspond to true edges in \( g \) and \( G \). This is done in such a way that a perfect combinatorial docking of \( s \) inside \( S \) constitutes the lowest energy state of the system. Thus imagine putting at the centers, \( \{\vec{R}(I) + \vec{R}(J)\}/2 \), of the edges in \( S \) for which \( C(I, J) = 1 \), positive, unit charges. Likewise, we put at all \( \{\vec{r}(i) + \vec{r}(j)\}/2 \) for which \( c(i, j) = 1 \), negative, unit charges. The total mutual interaction energy then is:

\[
U\{R(I), r(i)\} = -\sum_{I \neq J}^{N} \sum_{i \neq j}^{n} C(I, J) \cdot c(i, j) \{V(|\vec{R}(I) + \vec{R}(J) - \vec{r}(i) - \vec{r}(j)/2|)\}
\]

For any pairwise potential \( V(\rho) \) which is monotonically decreasing with \( \rho \) the absolute minimum of the interaction energy occurs when \( s \) has perfectly docked inside \( S \). This is when \( (\vec{R}(I) + \vec{R}(J) - \vec{r}(i) - \vec{r}(j)) \) vanishes for all

\[
C(I, J) \cdot c(i, j) = 1.
\]

Keeping \( S \) fixed at some standard position we let \( s \) move according the first-order dynamics (Eq. (4)) under the attractive, pairwise forces which derive from the above potentials. Since \( s \) is rigid, this motion consists mainly of rotations. This requires some relatively straightforward modifications with (anti-symmetric) tensor torques \( \tau(\alpha, \beta) \) and corresponding infinitesimal rotations \( \theta(\alpha, \beta) \) in the \( \alpha, \beta \) plane replacing vector forces and displacements:

\[
\theta_{\alpha\beta}(t + \delta) = \theta_{\alpha\beta}(t) + \frac{\tau_{\alpha\beta}}{\mu} \delta
\]

Imagine that we are performing all of this in \( (N-1) > (n-1) \) dimensions. To avoid any biasing we should place \( s \), at \( t = 0 \), in a position which is completely symmetric with respect to \( S \). Thus whatever non-symmetric movements of \( s \) eventually occur these will solely reflect—via the asymmetric forces/torques exerted on \( s \)—the asymmetric \( C(I, J) \).

Unfortunately we have \( \binom{n}{n} \) different ways of putting \( s \) at the center of \( S \) and orienting it parallel to any one of the \((n-1)\) dimensional “Faces” of \( S \) which are symmetric \( n \) (sub)simplexes each.
Since every such choice may bias the outcome of the dynamical evolution utilizing these particular initial conditions, we should repeat the process for each of the \( \binom{n}{\nu} \) different orientations, thereby clearly exhibiting a non-polynomial complexity.

This difficulty is avoided by formulating the problem in \( (N + n - 2) \) dimensions, the sum of the dimensions \( (N - 1) \) and \( (n - 1) \) of the embedding spaces of \( S \) and \( s \).

From the vantage point of the \( (N - 1) \) dimensional “Big” simplex \( S \), we are putting all of the simplex \( s \) at the only symmetric location, namely just at its center! We choose the latter to be the origin of the \( (N - 1) \) cartesian coordinate system: \( X(1), X(2),...,X(N-1) \). Now it is immaterial how we choose to orient \( s \) relative to the remaining \( (n - 1) \) coordinates: \( x(1), x(2),...,x(n-1) \) whose origin we again fix at the same common location. The point is that all the forces depend only on distances \( |\vec{R}(I) - \vec{r}(i)| \). By the Pythagorean theorem these depend initially only on sums of squares of \( x(i) \) and \( X(I) \) coordinates and are therefore invariant with respect to any rotation of the \( x(1),...,x(n-1) \) coordinate frame.

Once the torques due to the forces between pairs of edges in \( S \) and \( s \) start operating this initial symmetry will be broken and the system will evolve (mainly rotate) in the full \( (N + n - 2) \) dimensions. The energy is then a function of a large \( (N + n - 2) \cdot (N + n - 3)/2 \) number of rotation angles. We conjecture, but have not been able to yet prove, that, as in the case of translations, this large number of degrees of freedom avoids local minima of the energy. This would imply that the system persistently evolve in short time towards its absolute minimum. The latter is achieved on the “boundary” namely when all the corresponding vertices in \( S \) and in \( s \) overlap, and \( g \) has been found in \( G \).

Many NP complete problems correspond to special choices of the “small graph \( g \). Having all \( c_{ij} = i \neq j = 1...n \) corresponds to the problem of searching for a perfect clique of size \( n \) inside \( G \).

Taking \( (n = N) \) and \( c_{12} = c_{23} = ...c_{j,j+1} = ...c_{n-1,n} = c_{n,1} = 1 \), all other \( c_{ij} = 0 \)—i.e., having \( g \) which consists of just one cycle of \( (n = N) \) vertices—yield the Hamiltonian path problem; namely, of searching a Hamiltonian path in \( G \). The latter is a path in \( G \) consisting of edges \( E_{t_1,t_2} \) in \( G \), which visits all the vertices in the graph exactly one time. This is the simplest variant of the celebrated “Traveling Salesman problem” where all the distances between any pair \( g \) cities are the same, highlighting the purely combinatorial (rather than algebraic aspects) of this NPC problem.
IV. SUMMARY

We briefly describe a new deterministic, computational approach to complex problems and conjecture that the new approach may be applicable to NPC problems. In particular, we considered the problem of searching a graph \( g \) inside \( G \). Jointly with V. Gudkov we are presently testing the idea in concrete codes to see what is the real impact on some NPC problems. If successful, our approach will have many applications in quite a few areas. [1]

Acknowledgments

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[1] M. M’ezard, G. Parisi and M. A. Virasoro, Spin Glass Theory and Beyond (World Scientific, Singapore, 1987).
[2] T. A. Sudkamp, Languages and Machines: An Introduction to the Theory of Computer Science, Addison-Wesley, Reading, MA, 1997
[3] An analogous physical system was used by Farhi, Goldstone, Gutmann and Sipser, arXiv: quant-ph/0001106 (2000). Their idea was to create a wave function of \( n \) spins satisfying a set of Boolean logic requirements via adiabatic changing of the Hamiltonian.
[4] V. Gudkov, J. E. Johnson and S. Nussinov, arXiv: physics/02098011 (2002).
[5] V. Gudkov and S. Nussinov, arXiv: physics/02098012 (2002).
[6] For a specific convenient coordinate choice for the \( n \) vertices, see Appendix of Ref. 4.
[7] Strictly the analog of the first-order dynamics for translation (Eq. (2)) is \( \mu_{\alpha\beta,\sigma\nu} = \tau_{\alpha\beta} \) with \( \tau_{\alpha\beta} = \sum_{ij,ij'}(F_{ij}F_{ij'})\alpha(\rho_{ij})\beta - (\beta \leftrightarrow \alpha) \) the torque exerted by \( S \) on \( s \). The viscosity tensor \( \mu_{\alpha\beta\sigma\tau} \) reduces to a constant if we assume that the frictional forces act symmetrically at all the \( n \) vertices of \( s \). The last equations then becomes \( \tau_{\alpha\beta} = \mu_{\omega_{\alpha\beta}}. \)
[8] It appears (V. Gudkov and S.Nussinov, unpublished) that for this specific problem, even the "old" method of processing only the one original graph \( G \) may be applicable. We “tune” the ratio of strengths of the repulsive and attractive interactions. By using a ratio of order unity—which is considerably higher than the one previously used in Ref. 4, where we looked...
for clusters or “imperfect cliques”—we selectively collapse only (and hopefully all) the perfect cliques in the graph $G$.

[9] In this specific case, since we associate with both $G$ and $g$ symmetric ($n = N$) simplexes $S$ and $s$, we could put the simplex $s$ so as to literally overlap $S$ coexisting in the same ($N - 1$) dimensional space. The initially chosen orientation (or the labeling of vertices in $g$ used in the above definition of the connectivity matrix of $g$) will, in general, not correspond to the minimal energy. The simplex $s$ will then start rotating due to the forces constructed above relative to $G$ until the “combinatorially (= energetically) optimal” docking obtains. Since only the even permutations of $N$ elements can be achieved via continuous rotation we may need to repeat our search twice starting once with the simplex $s$ and once with $s'$. namely, $s$ in which one transposition, say, $V(1) \leftrightarrow V(2)$ has been performed.

[10] It has been argued that by studying neural nets and the human brain in particular, we may artificially emulate the versatility, pattern recognition and problem solving powers of the latter. We would like to suggest that the working of our brain is similar to that of our novel approach, though there is no analogue physical system there tuned to solve common problems. The highly inter-connected system of neurons has—unlike ordinary CPU’s and even more advanced special purpose “lattice” computers designed for specific physical problems (eg. nonpertubative QCD)—a high effective (Hausdorff) dimension. Also our distributed memory and the intuitive sensing of a complete “Gestalt” form strongly suggests a mode of operation with almost continuous, small, changes of many elements in parallel.