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POTENTIAL ENERGY SURFACES FOR CONCEPTUAL DESIGN AND ANALYSIS OF MECHANICAL SYSTEMS

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ABSTRACT

Current computational Design Synthesis approaches have had trouble generating components with higher kinematic pairs and have instead relied on libraries of predefined components. However, higher kinematic pairs are ubiquitous in many mechanical devices such as ratchets, latches, locks, trigger mechanisms, clock escapements, and materials handling systems. In many cases there is a need to synthesize new higher kinematic pair devices. To address this problem, we develop a new representation for mechanical systems that extends the capabilities of configuration spaces to consider arbitrary energy storing mechanical devices. The key idea underlying this representation is the use of potential energy surfaces as a generalization of configuration spaces. This generalization enables modelling of mechanical systems in a physics independent manner and captures behaviors such as dynamics. By modeling a device through the lens of a potential energy surface, we demonstrate that differentiable simulation is possible. Differentiable simulation enables efficient calculation of gradients of potential energy surface parameters with respect to an objective function that depends on trajectories taken on the potential energy surface. This allows synthesis of mechanical devices with desired kinematic and dynamic behavior through gradient descent. We demonstrate this through several synthesis examples including positioning devices (e.g., a funnel) and timing devices (e.g., an oscillator).

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INTRODUCTION

Current approaches to automated conceptual design of mechanical systems generally rely on building up a concept from a library of components. Concepts are built by connecting components together at defined connections, reparameterizing them, and/or replacing parts of a graph specifying higher-level function. However, these approaches can only synthesize concepts which contain these (preexisting) components. What if a higher-level function is needed—for example, a timing circuit—but there is no existing component or set of components that can provide this function? Or what if the planned usage environment is such that the existing components will not work—for example, in environments with high electromagnetic interference? In such cases, we would need to directly synthesize new mechanical components.

In this paper, we consider the conceptual design of a specific class of component, representative of rigid bodies which may move relative to each other, and which may also interact with springs and potential energy storage elements. While this might seem niche, a large number of useful mechanical devices such as ratchets, clock escapements, and trigger mechanisms are of this class. If we temporarily ignore the springs and potential energy storing elements, this class of mechanisms is traditionally called a *higher kinematic pair*. A higher kinematic pair consists of rigid shapes which may move relative to each other. Higher pairs can exhibit variable contact behavior leading to more interesting behavior than may be typically realized from gearboxes and linkages [1]. Higher kinematic pairs have important applica-

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tions in mechanisms such as ratchets, locks, latches, intermittent motion mechanisms, and escapements.

However, designing such higher kinematic pairs is difficult, particularly if you need a new type of, for example, clock escapement or a specific type of intermittent motion not well captured by an existing component library. One particular case for which it is difficult to use component libraries is materials handling. That is, machines which have flows of rigid bodies through them have higher kinematic pairs between the rigid bodies being flowed and the structures that guide and manipulate them. For example, a can in a vending machine and the structure that guides the can may be seen as a higher kinematic pair.

Designing a machine which has a flow of rigid bodies may require developing components specific to the rigid body being flowed and task being performed. Trying to capture such behavior—where the structure of the device itself plays an integral role in guiding part behavior—become prohibitive if only using mixtures of existing components in a library.

To address this challenge—both in terms of how to model this higher level kinematic pair behavior and how to design or optimize for it—this paper contributes the following:

1. We describe how to cast the design of higher order kinematic pairs as essentially an optimization over *Potential Energy Surfaces*. In doing so, we generalize classical approaches to analyzing higher kinematic pairs such as configuration space techniques, which we capture as a special case. This also extends to multi-physics regimes wherein physical contact between rigid bodies is not necessary, as it is in configuration space methods.
2. We demonstrate how casting mechanical devices as Potential Energy Surfaces can analyze existing rigid contact devices—e.g., trigger mechanisms—with the same accuracy as traditional Configuration Space (C-Space) methods, while also accounting for the effects of springs and energy storage devices that C-Space methods do not commonly account for.
3. We describe how this new representation of higher kinematic pairs permits direct optimization of its behavior that can leverage gradient-based techniques. Doing so allows us to specify high level objectives for a device's function (e.g., using an input torque to maintain oscillation in spite of damping), and automatically discover and optimize potential energy surfaces to meet that function. We accomplish this by casting the device motion and interaction with the underlying potential energy surface as a differentiable simulation upon which we can efficiently compute gradients.
4. We demonstrate the efficacy of this approach by directly optimizing for two types of common mechanical devices—funnels and oscillators—directly from first principles and without the need for predefining those devices or their components.

RELATED WORK

Automated conceptual design approaches have used library and graph grammatical approaches for synthesizing concepts. While some approaches have employed components that contained higher pairs, so far none of these approaches have generated higher kinematic pair devices. Approaches for generating higher kinematic pairs have been limited. Some are not automated, serving as an interactive design tool that requires user input. Others are capable of modifying devices which already exist to have better behavior or different configurations. Approaches that have generated higher kinematic pairs have generally produced fairly simple ones and only considered kinematic function rather than dynamic function.

Computational Design Synthesis for Conceptual Design

Kurtoglu et al. demonstrated an approach wherein graph grammars are used to construct a function structure from a black box which was then transformed into a graph of connected electromechanical components using another graph grammar [2]. However, it was difficult to determine if such concepts were valid and to evaluate the value of generated concepts with respect to each other. A number of automated conceptual design synthesis approaches employ construction of simulatable models which aid in the generation of valid and performant concepts.

Münzer and Shea demonstrated an approach for synthesizing concept model graphs [3] which were also valid bond graphs which could be simulated. Components were connected together using first order logic and boolean satisfiability. Many of these conceptual design methods do not generate components in geometric space, but there has been some success at generating certain classes of mechanisms such as gearboxes and linkages.

Radhakrishnan and Campbell demonstrated a graph grammatical method for synthesizing planar mechanisms such as linkages [4]. Kota demonstrated a means of synthesizing mechanisms to achieve desired kinematic requirements by assembling together building blocks such as linkages, gear pairs, pulleys, geneva mechanisms with defined geometric connection points [5].

The Geneva mechanism is an example of a higher pair kinematic device. Even though this approach employed a higher pair device it could not generate it. None of these approaches can be used to generate mechanical components with higher kinematic pairs.

Synthesis of Higher Kinematic Pair Devices via Configuration Spaces

Unlike the above methods, which largely focus on more defined kinematic synthesis of linkage or simple mechanisms, an area with many opportunities for mechanical conceptual design is that of higher kinematic pair devices. Before we proceed fur-

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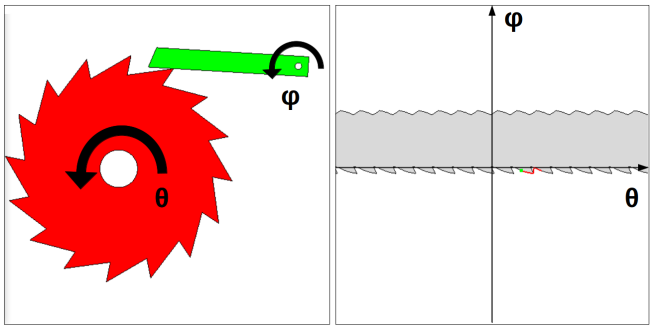

FIGURE 1: A ratchet(left) and its corresponding toroidal configuration space(right)

ther, we must understand how higher kinematic pairs may be analyzed, as it is necessary to understand related conceptual design methods.

It has been shown that higher kinematic pairs may be analyzed by considering their configuration space [1, 6]. A configuration space is a map in relative coordinates of each pair component showing whether the pair is intersecting, non-intersecting, or in contact. Regions of configuration space where the parts are intersecting are called blocked, non-intersecting; free, and in contact; boundaries. The relative motion of parts may be analyzed by considering trajectories in configuration space through free space and on the boundaries.

The configuration space approach can be difficult to apply in higher dimensions, but low dimensional (2D and 3D) configuration spaces are fairly versatile and may be used to describe a wide variety of mechanisms through composition of them. We shall consider 2D configuration spaces for now. With 2D configuration spaces, we can describe how two components may move relative to each other with respect to two translations, rotation and translation, or two rotations. The space of two translations exists on a plane, the space of a rotation and translation exists on the surface of cylinder, and the space of two rotations exists on a torus.

An example of a mechanism and its corresponding configuration space, which was generated using the HIPAIR software [7], is shown in Figure 1. The ratchet wheel rotates with angle θ and the pawl rotates with angle ϕ. As the ratchet has two parts which may rotate relative to each other this configuration space exists upon a topological torus and is periodic along both dimensions.

The configuration space method has also been employed for design. Caine [8] demonstrated an interactive design method that enabled a user to tailor 3D C-spaces(translation, translation, rotation) to have desired behavior. This was applied to the design of peg and hole devices and part orientation filters. The user could interact with features in C-space, leading to changes in the dimensions of the corresponding. It must be emphasized that changes were entirely manual. Kyung et al. [9] demonstrated a similar tool that allowed a parametric model to have its dimensions tuned to meet a required C-space. However, unlike the previous approach, this approach allowed the dimensions to be automatically modified until the desired C-space was attained.

Stahovich et al. [10] demonstrated how new designs may be synthesized from a sketch of a working mechanical device and its transition diagram. This technique used qualitative representations of configuration space and limited the number of possible directions of movement. A simplifying assumption of this approach is that inertia is ignored so it cannot take into account energy and power flow. Again, this approach could only resynthesize existing devices

Joskowicz and Sanjaya [11] showed how, given a configuration space and some constraints, one may synthesize simple shapes that have the specified configuration space. Slaboch and Voglewede [12] demonstrate an approach for realizing a specific type of configuration space and apply it to synthesizing planar variable kinematic joints. This was used to design concepts for adjustable plier mechanisms and swivel joints for a touchscreen laptop. Much more complicated shapes were realized, but this was only applicable for one type of device.

Li et al. [13] have shown how multi-state mechanical devices may be synthesized from a state graph by first synthesizing the configuration spaces of the pairs and then choosing appropriate pairs from a library. Only kinematic behavior was considered so inertia was not taken into account. Generated C-spaces were fairly simple because movement was only considered to be possible in 8 directions.

Unlike past approaches to both computational design synthesis and configuration space design, this paper generalizes some of these approaches in important ways. For example, the proposed approach provides a principled way to handle non-rigid-body-contact in a structure (say from magnetic fields or flowing continuum fields). Likewise, because it does not depend on parameterized component libraries, it can create components with unique topologies. In addition, it can be used to design components with dynamic function.

CONTRIBUTION 1: POTENTIAL ENERGY SURFACES AS A MECHANICAL DESIGN REPRESENTATION

To clearly motivate and describe how and why Potential Energy Surfaces (PES) provide a reasonable generalization of Configuration spaces for mechanical design, it is illustrative to consider why certain machines are hard to describe using configuration spaces. From this, we can build up an understanding of how potential energy surfaces resolves some of those difficulties.

Many mechanical devices like an escapement or a ratchet cannot be described purely with with configuration spaces due to the presence of springs or a similar gravitational restoring force. In fact, energy storing elements are necessary so that many

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higher pair devices can perform their function. For example, a ratchet cannot work without a spring or weight to restore the ratchet pawl. C-Space methods do not commonly consider or model these energy storage mechanisms directly, but are naturally modeled by the type of potential energy they store.

These energy storing elements, such as springs, have different values of potential energy according to the relative positions of parts of the mechanism. So, instead of describing only rigid contact, we can assign each point in space to have some value of potential energy according to the potential energy provided by the corresponding energy storing element. However, we must find some way to handle the potential energy of the kinematic pair. We do so by considering blocked regions to have *infinite* potential energy and free regions can be considered to have zero potential energy as was considered by Bennett [14] in his hypothetical Brownian Mechanical Turing machine. These free regions can be considered to have the potential energy given by the deformation of any attached springs or potential energy storing devices attached to the mechanism. We call this representation a *potential energy surface*.

Potential energy surfaces are an idea used in chemistry for describing the behavior of molecules and chemical reactions [15]. We can consider the energy of a molecule at each point in a given coordinate system. For example we may have a coordinate system defined by using the length of one bond as the x coordinate and the length of the second bond as the y coordinate. We can even define a coordinate system from the relative angles or displacements between only the groups we care about in a molecule, allowing us to describe the behavior of these two groups in a lower dimensional space than the relative angles and displacements between all atoms in the molecule. This allows us to carry out useful analyses of molecular behavior in lower dimensions. Minimum energy paths on potential energy surfaces can be used to determine the likelihood of chemical reactions.

As stated before, configuration spaces can map directly to potential energy surfaces, as blocked regions can be considered to have infinite potential energy. While true in principle, for a variety of practical and computational reasons, it becomes useful to relax this assumption. For example, to aid in simulation stability, it is helpful to have a smooth increase of energy from free to blocked space, or to consider that blocked space has a finite, but very, large potential energy. This work uses the artificial potential field method from robotics to convert C-space geometry into a potential energy surface representative of the original configuration space, but which also exhibits smooth transitions between blocked and unblocked regions [16, 17]. Specifically, the potential energy is calculated as:

$$E = \begin{cases} \frac{v}{2}(\frac{1}{r} - \frac{1}{r_c})^2, r < r_c \\ 0,\ r > r_c \end{cases} \quad (1)$$

Where r is the minimum distance from a point to blocked space and r_c is the cut off distance to which potential energy goes to zero. These parameters should be chosen depending on the size of the simulation time step. While this is an approximation, we note that real devices are not rigid bodies, so there will be some small deformation of both parts. The resultant potential energy surface may be summed with the potential energy surface induced by springs or other energy storing media attached to the mechanism to make a potential energy surface representative of the whole device.

For this paper, we shall consider the 2D case for the time being with potential energy being a function of two relative displacements, two relative rotations, or a relative displacement and relative rotation, since this captures the most common forms of higher kinematic pairs.

SIMULATING POTENTIAL ENERGY SURFACES

As described above, we define a 2D potential energy surface as a set of values of potential energy on a plane, cylinder or torus. Specifically, we define our potential energy surfaces by a 2D rectangular grid of points at which potential energy values are assigned. We determine potential energy values between those points via bilinear interpolation. For a toroidal potential energy surface, both axes are periodic, so the grid wraps around on top/bottom and the sides. For a cylindrical potential energy surface one axis is set to be periodic and wraps around on either the sides or top/bottom. For a planar potential energy surface neither axis is set to periodic.

In a manner similar to the analysis of motion in configuration space, we can consider how a particle—a set of relative displacements equal to the dimension of the potential energy surface—moves on the potential energy surface under the action of an external force applied to the particle and force applied by the potential energy surface, which is the gradient of potential energy. These external '*forces*' correspond to forces in the case of a potential energy surface determined by two translations, two torques in the case of a potential energy surface determined by two rotations, and a torque and force when the potential energy surface is defined by a rotation and translation. We may consider how the particle moves on the surface in a quasistatic manner, by translating the particle by an amount proportional to the net force at the current position. We can assign an inertia value to each axis and integrate forces applied from the potential energy surface and external forces to calculate a *trajectory*, which considers dynamic behavior. For stable simulation we have found it necessary to add a damping function so that the particle does not accelerate infinitely. Note that that the damping function may be different for both axes. For the dynamic case we use velocity Verlet integration with linear damping, which is summarized

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FIGURE 2: A spring loaded dart gun

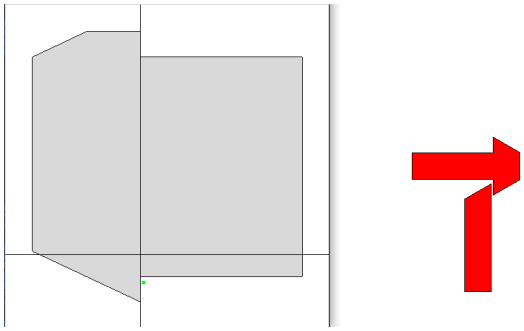

FIGURE 3: Dart Gun Mechanism C-space

below:

$$X_{n+1} = X + \Delta_t V + \frac{F_n \Delta_t^2}{2m} \tag{2}$$

$$V_{n+1} = \frac{1}{1+\Delta_t \gamma/2m}[V_n(1-\Delta_t/2m) + \frac{\Delta_t}{2m}(F_{n-1}+F_n)] \tag{3}$$

We note again that m and γ may be a vector of inertias or dampings equal to the dimension of the potential energy surface. For the case of non-periodic potential energy surfaces such as those on planes or cylinders we must specify how particle collisions with the boundary are handled. We use a method similar the modelling of walls in molecular dynamics, as this conserves energy better than translating particles that exit the simulation box back in with reflected velocity [18]. If a particle is within some distance of the wall, a spring force is applied proportional to the distance the particle is inside the wall.

CONTRIBUTION 2: POTENTIAL ENERGY SURFACES FOR ANALYSIS

Here we show how a potential energy surface may be used to describe, model, and analyze a mechanical device in a physics-independent manner. Consider the device shown in Fig. 2, which consists of a spring loaded dart and a trigger assembly which guides the dart and interfaces with the user to control dart release.

Many simple dart toys employ this mechanism, although this mechanism finds use elsewhere, most often where mechanical energy needs to be stored and quickly released. We will show that the above device's function can be almost entirely described with one potential energy surface. We can simplify the device into two parts: the dart and the trigger. We can consider the dart to be restricted to move horizontally along the x axis and the trigger to move vertically along the y axis. Since we have two parts which are capable of translation with respect to each other we have a planar translation-translation c-space. We show a simplified view of the dart and trigger mechanism and their respective C-space, which was generated with HIPAIR [7], in Fig. 3. For purposes of clarity, the potential energy surface shown only considers dart displacement up until the point the dart spring reaches equilibrium.

Some customer needs of dart blaster toys include: shoots darts a long distance, lightweight, entertaining dart flight, easy to reload, and easy to fire dart. [19] Paths in the potential energy surface allow us to quantify some of these customer needs. We can determine if the reload action can be carried out with an acceptable amount of force by applying a horizontal force of desired magnitude in the positive X direction to a particle for a set amount of time. The resulting path during a successful reload operation is shown in Fig. 4. As we can see from the successful trajectory, the particle eventually reaches equilibrium after force stops being applied. This allows us to quantify the "ease of reloading" customer need. We must admit that reloading involves actions other than just pushing the dart back and may include picking up the dart and aligning it, however such actions are beyond the scope of this method.

We can also simulate what happens when the user carries out the fire dart function. We can apply a force for a set amount of time in the downward direction with the desired magnitude to a particle which starts at the equilibrium position we found in the previous step. The resultant trajectory is shown in Fig. 4. The horizontal speed the particle achieves when it exits the potential energy surface directly relates to the customer need of firing darts a long distance. We must also note that one might employ a more complicated means of applying force to the particle to simulate action by the user.

The potential energy surface also helps us place bounds on how small we can make the device. For example, given that we have a translation-translation potential energy surface, translations on the potential energy surface correspond to relative translations in real space. In order for the device to function it must at least contain the trajectories taken by a particle during the reload and fire functions. And while there are exotic options like using electric, magnetic, and pressure fields to achieve a function of po-

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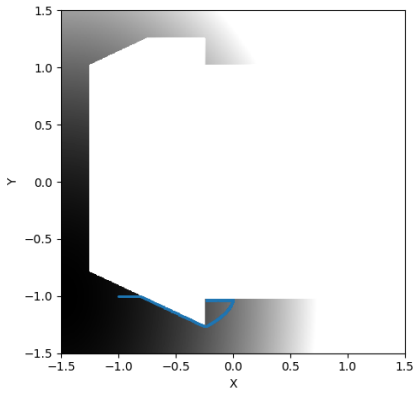
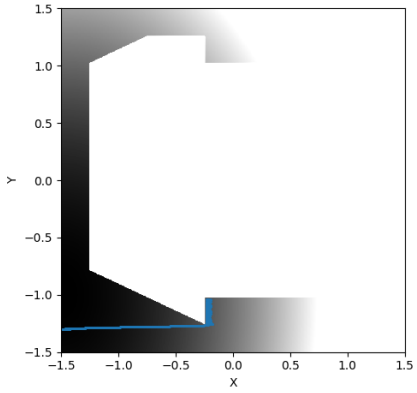


(a)



(b)

FIGURE 4: (a), path through PES during load, (b) path through PES during trigger

tential energy while the dart is outside of the geometric bounds of the device these are probably impractical due to applied forces generally decreasing with distance from elements which produce them. Shrinking the potential energy surface also reveals a conflict between making the device smaller and ease of reloading. While a smaller potential energy surface can impart the same amount of kinetic energy to the dart, the gradient and force the user must overcome to load the device is larger.

In this way, analyzing devices by their PES provides more insight into possible functions than through C-Space analysis alone.

CONTRIBUTION 3: SYNTHESIS OF POTENTIAL ENERGY SURFACES

We define a potential energy surface with a grid of parameter values p, which was transformed into a grid of potential energy

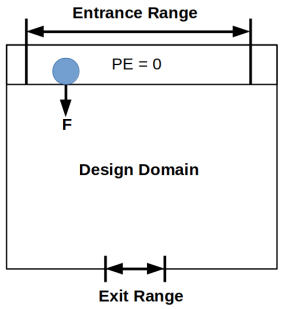


FIGURE 5: Description of Funnel Problem

values with the following equation:

$$PE_{ij} = E * p_{ij}^2 \tag{4}$$

E is an arbitrarily chosen constant for adjusting the range of possible energy values. This function also ensures that the potential energy will always be positive. While, there are phenomena that allow the potential energy of the potential energy surface to be less than the environment(IE magnetic attraction), we do not desire a potential surface with negative potential energy relative to the environment in this case. If we desire negative potential energies we may uniformly subtract some energy value from all grid points of a potential energy surface that consists of only positive values, with the energy value being such that some parts will be negative. The grid of potential energy values is gaussian blurred to smooth out transitions in potential energy.

We develop a method for automatically designing potential energy surfaces based on gradient descent. This is possible because we can automatically differentiate our simulator using Autograd [20] which enables us to calculate the gradient of our objective function with respect to potential energy grid values. By keeping track of which numerical operations were used to arrive at a result, it is possible to obtain derivatives of that result with respect to the inputs. The Autograd library enables the differentiation of native python and numpy code written in the appropriate format. Using Autograd, it is possible for us to differentiate back through an objective function that depends on particle trajectories, through each simulation step that moves the particles with with Verlet integration, back through our gaussian blur function, and back to each grid value of potential energy to get the gradient of the objective function with respect to energy of each grid value.

We note that, in most cases we should use multiple particles, preferably with differing initial conditions or per-particle random noise, so that particles take a wide variety of trajectories on the potential energy surface. This way we get particle trajectories that visit more parts of the surface, because unvisited parts of the potential energy surface have no influence on the particle trajec-

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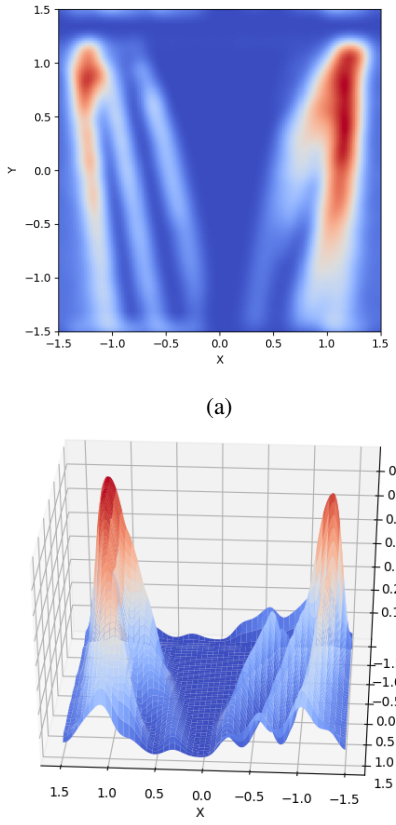
tories, the gradient with respect to the particle trajectory will be zero at these locations.

Consider the problem of designing a potential energy surface for manipulating material that acts like a funnel. One problem we often face when moving material around is accepting material which has a large range of possible positions and reducing the range of possible position values. When handling material at various steps we may need the position of the material to be within a certain range, as is the case in an assembly machine which requires various components be in the correct place so that they may be assembled. However, the material coming into the system may not necessarily have the correct positioning. The system we design will take in objects within a range of x values at the top of the domain and will cause them to exit the domain within a smaller range of x values at the bottom of the domain. A constant downward force is applied to all objects to drive them through the domain. In order to get a better estimate of the gradient, we should use multiple particles. Our objective function is to minimize the objective function which was summed at every time step:

$$obj = \sum_{i=1}^{n} (x_i - x_0)^2 \tag{5}$$

where x_i is the final x position of the ith particle and x_0 is the desired x value of particles exiting the domain. x_0 in this problem was chosen to be zero, the center of the domain. We start our particles at random x positions at the top of the domain in a region which is set to zero potential energy. This models a region outside the funnel design domain where the particles start. This prevents the the optimization from starting the particles at the top of slope to sling them toward the center of the domain. In addition to the constant downward force, we also apply a relatively small random noise force to each particle. This helps with exploration by pushing particles into regions they would otherwise not visit and thus obtain non-zero gradients for more grid values.

We use a 200x200 grid of values which was transformed into a potential energy surface in the aforementioned manner. Grid values were initialized to a small random value to break symmetry and ensure gradients would be non-zero. Gradient descent was carried out using RMSprop. This acts like stochastic gradient descent because of the random noise force we add to the particles at each time step. One reason for using RMSProp as opposed to other algorithms is that it can handle very large gradients by adapting the learning rate. The gradients of particle trajectories with respect to an objective function, may in some cases be very large. One reason for this is that unlike topology optimization of structures where we have constraints on the amount of material we use, there is no need for constraints on potential energy. In fact, if we desire a structure that approximates a kinematic pair, we desire the potential energy to go to infinity. For example, recall that blocked regions in C-space can be seen as regions of infinite potential energy. So, in fact, if we wish to find a potential energy surface which can be easily translated to a configuration space, we desire regions of very high potential energy which approach infinity. To aid in the stability of the gradient updates, one could employ either gradient clipping methods or Trust Region methods, such as in Trust Region Policy Optimization, to make these policy updates more gradual.



(a)

(b)

FIGURE 6: Funnel Potential Energy Surface

Results

We obtain a potential energy surface that works like a funnel as shown in Fig. 6. Similarly to a funnel, it has two diagonal regions of high potential energy surrounding a region of low. As shown in Fig. 7, particles which enter the top of the domain end up near the center of the domain. Arriving at this result took 5700 iterations.

The inside of the funnel is largely at zero potential energy which is important so that particles may enter the funnel. There are some spurious particle trajectories, but it is possible that

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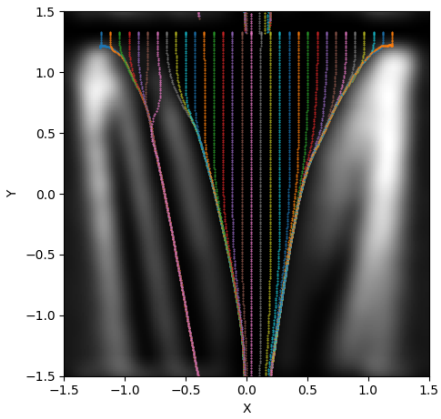


FIGURE 7: Particle Paths on optimal potential energy surface

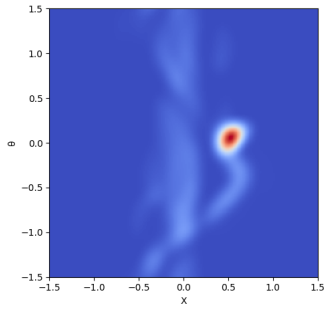
smoothing approaches could remove them. This is, however, a conceptual design for a funnel that may be further refined during realization of the funnel.

CONTRIBUTION 4: EXAMPLE OF SYNTHESIZING AN OSCILLATOR

Consider the problem of designing a device to keep a pendulum or mass on a spring oscillating in the presence of damping using an input torque with some amount of variation. This is similar to the problem of designing a clock escapement except without the restriction that rotation of the supply torque must complete a rotation at a near constant rate. Designing an oscillator is a dynamic rather than kinematic problem, which is something previous approaches have not yet been able to synthesize. For this problem we assume a cylindrical potential energy surface. We apply a variable torque which ranges between a minimum and maximum value and are applied downward on the Y axis.

We assume for this problem that the oscillator operates in conjunction with a linear spring with equilibrium point at X = 0 attached to the x axis. We must note that the method developed here could probably discover the need for a spring, however, this simplifies optimization. We assume that our mechanism has much higher damping for motion in the Y-axis than motion in the X-axis. This is necessary so that oscillation in the x-axis has a relatively high q-factor and near free oscillation is possible. We must specify some means of evaluating oscillator mechanism performance that ideally must be measurable at each simulation time step. We develop a cost metric to be minimized that considers the RMS square of distance of all particles from the trajectory an undamped mass takes in phase space.

$$Cost = \frac{\sqrt{\sum_{i=0}^{n}(x_i - Acos(\omega t_i))^2 + (\dot{x}_i + A\omega cos(\omega t_i))^2}}{n^2} \quad (6)$$



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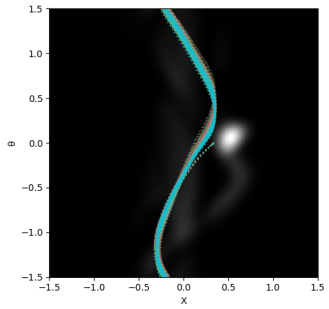

(b)

FIGURE 8: Synthesized potential energy surface(a) and particle Paths for synthesized oscillator(b)

We sum this cost metric for all timesteps of the simulation. A is the target amplitude and ω is the target frequency, and n is number of particles. In the simulation, particles are initialized at y = 0 with a larger X-value than the target amplitude to give the oscillating mechanism a starting kick. In addition, each particle is displaced from this starting amplitude by a small amount of random noise. This in addition to the randomly applied downward torques on the particles helps to ensure that each particle takes a slightly different path. More different paths mean that more grid points contribute to a particle's behavior, thus we can obtain the gradient with respect to them. Adding noise also helps make a device that is more robust to disturbances. In addition we also add the following regularization to the cost:

$$Regularization = R\sum_{i=0}\sum_{j=0}(E_{ij})^2 \quad (7)$$

Where R is the regularization factor and E_{ij} is the value of potential energy at a grid point. The regularization factor assists in smoothing out the potential energy surface and helps prevent the gradients from growing very large.

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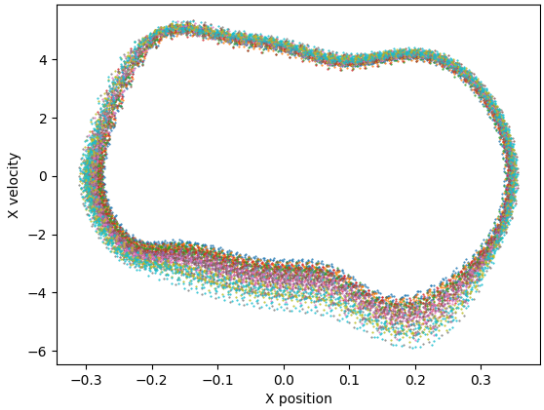

FIGURE 9: Particle trajectories in phase space, same start position, varying torque

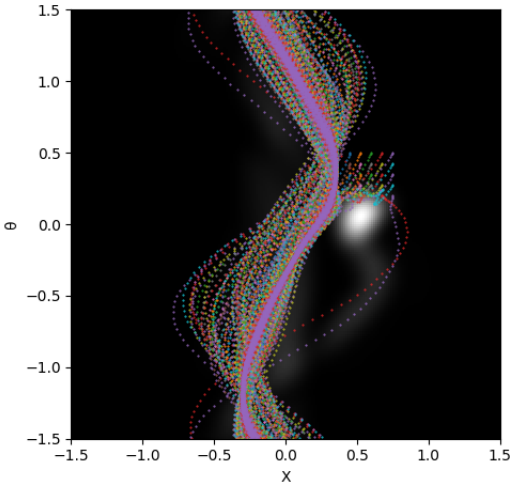

FIGURE 10: Particle paths for particles starting at a grid of positions

Results

A potential energy surface that displays a limit cycle when combined with a spring potential is found after 29400 iterations. Fig. 8 shows the trajectory taken by 50 different particles, each with a torque ranging from minimum torque to maximum torque. Particles were initialized at y=0 with an X value at the target oscillation amplitude. Figure 9 shows the plot of particle trajectories in phase space after three oscillation periods. The trajectories shown have a continuous loop indicating stable oscillation.

In addition, there are a number of other initial positions which result in the particles converging to the same trajectory in

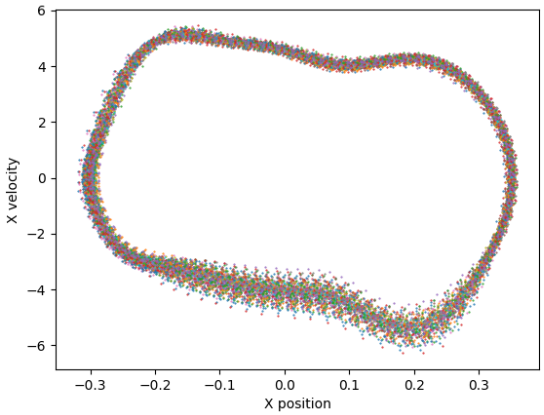

FIGURE 11: Trajectories in phase space that particles starting at a grid of locations eventually attain

phase space. Figure 10 shows the path taken by particles which were initialized in a 5x5 grid of initial positions with zero velocity and to which the maximum design torque is applied. The trajectory in phase space these particles take after 15 oscillation periods is shown in Figure 11. This is similar to the trajectories taken in Fig. 9. This indicates that the developed limit cycle is somewhat robust.

DISCUSSION

The potential energy surface representation allows devices containing a pair of rigid bodies which move relative to each other and springs to be described by a single representation. Potential energy surfaces allow a device's behavior to be modelled. In addition, we showed how potential energy surfaces can be optimized to exhibit desired behavior. The advantage of working in potential energy space is that we may determine 'how' to accomplish a given task before deciding what components or even what type of physics we should use.

One interesting property of potential energy surfaces is that they allow us to explore design alternatives. Potential energy surfaces need not correspond only to rigid bodies connected to springs—they can also be realized by other potential fields. For example, we could use highly compliant contacting components (as in soft robotics), or electric and magnetic fields, or a fluid pressure field in potential flow. We can even take advantage of potential fields in the environment, such as gravity, to realize part of a potential energy surface.

Potential energy surfaces also have some interesting implications for describing the function of mechanical devices: it implies that function may be represented in not only a form independent manner, but also a physics independent manner. While

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making analogs of mechanical devices using fields other than those realized by nearly rigid bodies may seem counterproductive, there may in fact be good cases for doing so. For example, by replacing rigid components with potential fields we may avoid wear, friction, and contacting components. In space systems, by avoiding contacting components we can avoid cold welding, which has been responsible for the failure of some mechanical systems in space.

More practically, in some cases switching to potential fields can offer higher performance. An example of this is a magnetic escapement developed by De Bethune which can achieve oscillation frequencies up to 1000 Hz. This is much faster than the 5 Hz beat frequency realized by a typical mechanical watch. Higher clock frequency translates to being able to measure time in smaller increments and less clock drift.

While this paper does not address how a potential energy surface may be mapped to fields that generate them, Xu and Virgin have experimentally demonstrated that a physical ball on 2D surface under gravity can approximate a planar potential energy surface [21]. Potential energy surfaces on cylinders might be approximated using a mechanism similar to barrel ballistic cams used in mechanical fire control computers. This mechanism consists of a barrel shaped cam which is free to rotate with a rolling ball follower on a lever pressed onto the surface of the cam with a spring and able to move axially along the length of the cam.

The current approach is readily generalizable beyond the funnel and oscillator design problems: you need only specify an appropriate metric of machine performance to be maximized or minimized that you can evaluate from particle trajectories, ideally at every simulation time step. In our current implementation it is not too difficult to formulate simulations where time varying forces are applied to particles and where particles have varying properties such as mass or damping. We do note that it can be difficult to formulate objective functions for multi-state design problems. For example, the aforementioned dart gun problem has states of loading, nothing happening, and firing. The current simulation approach might be coupled to other differentiable simulation engines [22] [23] to synthesize potential energy surfaces which are coupled to rigid bodies and soft bodies.

The primary limitation of this potential energy surface approach is that contact friction cannot be modelled. Potential energy surfaces cannot take into account how friction force depends on normal force, that friction force is perpendicular to contact, and that the location of contact matters. Configuration space approaches share this limitation.

In addition, mechanisms such as linkages that trace out a self-intersecting path cannot be described with potential energy surfaces. A single potential energy surface cannot enforce a particle to take a 1 degree of freedom path with a self intersecting loop under arbitrarily applied forces and at equal potential energy. We have shown that there are trivial ways to realize potential energy surfaces, but future research is needed to realize non-trivial potential energy surfaces. We have also yet to develop formal rules for describing how potential energy surfaces can be combined and interact with each other, so as of right now this approach can only describe single 2D potential energy surface devices.

CONCLUSION

This paper demonstrates how potential energy surfaces may be used to describe and synthesize machines. Potential energy surfaces extend the configuration space method to take into account energy storing behavior and describe entire machines with one representation. We showed how to model an entire mechanical device with one potential energy surface, demonstrating the discovery of simple mechanical devices like funnels and oscillators. Moreover, potential energy surfaces enable machine concepts to be computationally synthesized from an objective function that is a function of particle trajectories on the potential energy surface. The gradient of potential energy values with respect to the objective function can be obtained using automatic differentiation enabling synthesis of potential energy surfaces through gradient descent. This can not only be used to synthesize potential energy surfaces that solve kinematic problems, but problems which take into account dynamics. While more work remains on how to realize potential energy surfaces, potential energy surfaces offer a new avenue for solving problems with which past computational design synthesis techniques have struggled.

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