Colloidal information engine coupled to correlated active baths

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Abstract

During my summer internship at the Simon Fraser University, under the supervision and guidance of David Sivak and Johan du Buisson, I explored how information engine performance varies with the correlation structure of some coupled active noise. That is to say, which values of noise strength and correlation time optimise the rate at which the engine's operation extracts and practically stores free energy (the free power output) through the rectification of fluctuations. Two correlation structures were investigated in the simulations implemented here, labelled as the AOUP and PLOUP noise models. The results imply more strongly correlated noise only benefits free power output when the variance of active noise fluctuations is independent of correlation time; this is the case for PLOUP noise. The variance of AOUP noise is inversely proportional to correlation time. Thus, the white noise limit maximises free power then due to ever increasing fluctuation magnitudes in said limit. For both noise models, increasing the parameter associated solely with active noise magnitude increases the outputted free power.

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Contents

1 Brief introduction to molecular machines

The existence of complex life as we know it depends entirely upon the functioning of biological molecular machines. These are a diverse group of proteins which together perform the necessary tasks for cell operation. An example of a bipartite molecular machine (MM) is FoF1-ATP synthase, which operates within the mitochondria of all eukaryotes, using the proton gradient established by respiration to produce Adenosine triphosphate (ATP). This latter molecule is crucial for the storage and usage of energy within our cells. Other examples of MMs include RNA polymerase, digestive enzymes, and molecular motors such as Kinesin and Dynein which transport cellular cargoes along the microtubules of cells.

What makes researching molecular machines so interesting is their capacity to operate in conditions completely foreign to our everyday experience. We say that microscopic machines have a very low Reynolds' number, a quantity defined as,

$$Re = \frac{\rho_{fluid} v L}{\eta}\,, \tag{1}$$

where ρ_{fluid} denotes the the density of the fluid medium in which the MM operates, v is the flow speed, L a characteristic length of the MM, and η the medium's dynamic viscosity. The low Re implies that viscous forces the MMs are subjected to dominate over inertial forces to the extent that driven machines have effectively zero memory of their motion once said drive is removed. Therefore, MMs cannot rely upon momentum to complete operational cycles, like how macroscopic machines can exploit flywheels. Furthermore, a traditional heat engine uses a temperature gradient to extract useful work, however no such gradient exists within the isothermal cytoplasm of a cell. As a consequence, molecular machines must harness novel approaches for powering their operation. For such minute machines, the heat exchanged in thermal fluctuations is a substantial factor larger than the energy acquired per hydrolysed ATP [1]. Naively then, one would question the potential for MMs to serve any useful purpose, and yet they clearly do. Thus, a hallmark of transport MMs is their ability to rectify fluctuations from their surrounding environment to manifest directed locomotion.

The prospect of building practical artificial molecular becomes increasingly likely as our nanotechnology advances. Fortunately, natural selection has acted by proxy as invaluable research into optimal MM design. The pervading approach then to forming a theory of molecular machine operation is through the scrutiny of biological MMs, which demonstrate remarkable efficiencies compared to current artificial MMs. The mention of molecular machines provides relevant background to this discussion of information engines since such mechanisms offer a possible framework for elucidating biological MM operation. Within a cell, fluctuations may be too slow for the noise they produce to be deemed white. This noise is instead coloured and may have an exponentially decaying autocorrelation, like the noise models explored in this project.

2 What is an information engine?

A system in the absence of any feedback will relax from its initial conditions into the equilibrium state. This minimises the system's free energy and so no useful work is extractable, unless a specific feedback protocol is implemented which can exploit measurements of the current state. Information engines use information gathered by such measurements to favourably evolve some work parameter of the system and perform work.

The gedankenexperiment that introduced that concept of information engines was Maxwell's demon. A conscious demon was proposed that could measure the position and momenta of particles in an isothermal gas and use a frictionless trap door to separate them, without doing work, in such a way as to create a temperature differential. This could then be used to power a heat engine, therefore extracting work from an isothermal gas. This is an information engine as the demon's responses to measurements reverse the probabilistic tendency towards entropy maximisation and produce a low entropy configuration of particles, which is harnessed to do work.

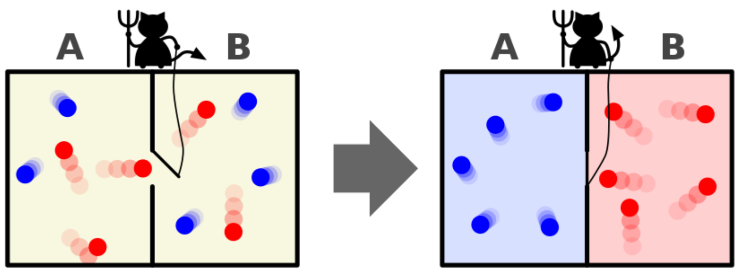

Figure 1: Diagram illustrating James Clerk Maxwell's "demon" [2].

Another paradigmatic information engine is Szilárd's engine. This consists of a feedback controller which measures which side of a movable partition a single gas particle resides within a two compartment container. The compartments contain either free space or a gas particle, so a pressure differential exists. The information gathered through measurement is used to reliably attach a piston to the opposite compartment of the particle; the expanding single particle gas then does work on the piston, and so information is converted into work here also.

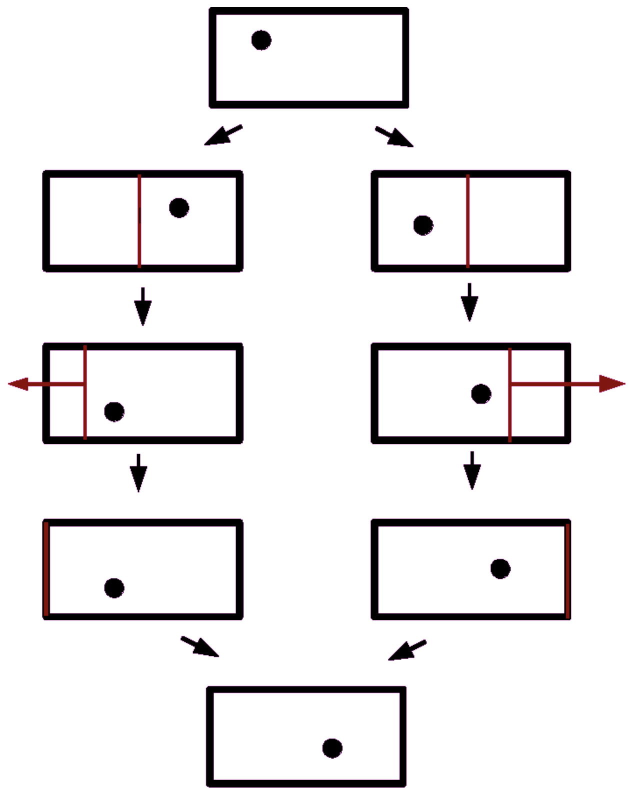

Figure 2: Diagram of Leó Szilárd's engine [3].

Despite thermal reservoirs being isothermal, systems coupled and equilibriated to them still experience thermal fluctuations. However, these fluctuations average out to contribute no net effect on the system. The purpose of an information engine is to measure the current system state, due to recent fluctuations, and update the equilibrium of the system to extract the fluctuations energies. The same principle of rectifying fluctuations applies also to active noise sources, as demonstrated by the colloidal information engine of interest here.

3 Theory for colloidal information engine

The experimentally realised information engine under consideration consists of a colloidal particle, vertically confined by optical tweezers. These tweezers are labelled the trap and produce a harmonic potential of effective stiffness κ. Feedback introduces unidimensionality into the colloid's evolution over time; the trap center ratchets upwards in response to the measurement of favourable, upwards, thermal fluctuations, acting to store free energy in the gravitational field over time [4].

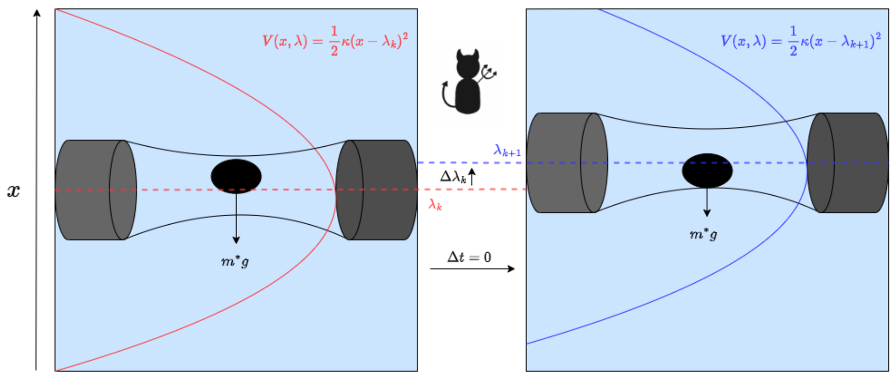

Figure 3: The apparatus above depicts an experimental realisation of the colloidal information engine. Optical tweezers confine the particle vertically until it is measured fluctuating above the trap center by the demon and its state is exploited in a ratchet event. This is when the trap position is shifted vertically upwards by some amount $\Delta\lambda$, whose magnitude is determined by the choice of feedback scheme. Ratcheting the trap converts information of the particle's state into free energy stored in the gravitational field.

3.1 Introduction to stochastic differential equations

First, we introduce some key concepts within stochastic calculus before returning to the information engine model. A stochastic differential equation (SDE) in x differs from an ordinary differential equation (ODE) in x by the addition of at least one random variable, known as noise. This causes the previously deterministic evolution of x to become stochastic; the SDE's solution is itself a random variable, whose statistics are defined by the nature of the equation. The general functional form for linear SDEs, written in terms of differentials, is,

$$dx = f(x,t)dt + g(x,t)\xi(t)\,, \tag{2}$$

wherein the first and second terms are named the drift and diffusion terms respectively. The name of the latter reflects the appearance of such terms during the analysis of Brownian motion, in which microscopic particles are seen to continually diffuse through their medium in response to stochastic collisions with that medium. In the case of Brownian motion, within a given experimentally observable period of time, the colloidal particles experience a vast number of collisions with the medium. Such collisions are synonymous with heat exchange between these particles and their surrounding medium, which is acting here as a thermal reservoir. Provided each instance of noise is independent, regardless of physical origin, the central limit theorem demands that the sum of these many collisions produces effective Gaussian noise. It can be shown that the sum of

Gaussian random variables is also Gaussian and thus, over time, exposure to exclusively Gaussian noise produces Gaussianly distributed observables.

What functional form should $\xi(t)$ take so as to produce Brownian motion? Firstly, we assume noise events are IID variables, meaning that they are independent and identically distributed. Their independence means that the correlation between noise at different times must be zero. This is reasonable under the assumption that many collisions will occur during finite experimental time intervals, as these subsequent collisions cause the particle to "forget" the nature of the noise at the previous measurement. We call independent noise (i.e. with zero correlation time) white noise due to its corresponding flat power spectrum; all frequencies contain equal power. Noise which is both Gaussian and white is often referred to as Brownian noise. Intuitively, for a particle subjected to solely white noise, the probability of diffusion in one direction should be equiprobable to diffusion in the reverse direction. As a consequence, one expects the noise's mean to be zero. Pivotally, upon subjecting a particle to white noise, the variance in its state should increase as the elapsed time increases because it has had longer to diffuse away from its initial state. In fact, the variance of the Brownian stochastic integral (a sum of all contributing Gaussian white noise events) must equal the time period elapsed. The combination of all these properties leads to the definition of a Wiener process.

So, the choice of $d\xi$ needed to reflect the infinitesimal influence of thermal fluctuations is proportional to dW, the Wiener increment. This differential has the following properties:

$$\langle dW \rangle = 0\,,$$
$$\langle dW_t\, dW_{t'} \rangle = \delta(t-t')\, dt\,,$$

where the δ seen in the Wiener increment's autocorrelation denotes a Dirac delta function. The diffusion term for an SDE characterising Brownian motion will consist of such a Wiener increment, with some prefactor accounting for the noise magnitude.

An Ornstein-Uhlenbeck (OU) equation is a simple class of SDE containing only additive noise. This means noise which does not directly depend upon the state of the system; it can only depend upon the current time elapsed (e.g. for equation (2) to be an OU equation, the diffusion term must contain no explicit x dependence). All SDEs seen in this review yield OU processes.

3.2 Gaussian bath Langevin equation

Consider a colloid confined by a stationary trap, i.e. confined in the absence of any feedback protocols. To identify possible trajectories taken by the system, one must solve the stochastic equivalent of Newton's second law, known as a

Langevin equation. The Langevin equation for the position x of a mass m particle, submersed in a fluid thermal reservoir, of density ρ_{fluid}, is given by,

$$m\ddot{x}(t) = -\gamma\dot{x}(t) \; - \kappa\Big(x(t) - \lambda(t)\Big) - mg + \frac{4}{3}\pi r^3 \rho_{fluid}\, g \; + \; \sqrt{2\gamma K_B T}\, \xi(t)\,. \quad (3)$$

The first term on the right-hand side gives the frictional contribution to the resultant force, with Stoke's law giving $\gamma = 6\pi\eta r$ for a spherical colloid of radius r moving through a fluid of dynamic viscosity η. Other contributions include the restorative force provided by the trap of stiffness κ, the colloid's weight and the upthrust in accordance with Archimedes' principle. The final term encapsulates the sum of forces imparted at time t due to random kicks from the thermal reservoir.

For simplicity's sake, the weight and upthrust will be combined into a single weight corresponding to some effective mass,

$$m^* = \frac{4}{3}\pi r^3 \big(\rho_{fluid} - \rho_{colloid}\big)\,. \quad (4)$$

A further simplification arises after recognising the particle's inertial timescale is about 6 orders of magnitude smaller than the timescale associated with particle relaxation in the trap. This condition is equivalent to having a low Reynolds' number as detailed in Section 1. Therefore, from hereon the Langevin equation's inertial term is regarded as negligible, giving a simpler, over-damped, Langevin equation:

$$\gamma\dot{x}(t) = -\kappa\Big(x(t) \; - \lambda(t)\Big) - m^* g + \gamma\, \sqrt{2D}\, \xi(t)\,. \quad (5)$$

In the diffusion term, the Stoke-Einstein equation,

$$D = \frac{K_B T}{\gamma}\,, \quad (6)$$

has been used, in which D symbolises the diffusion coefficient/noise strength.

3.2.1 Nondimensionalisation of the equation of motion

To reduce the number of parameters required when simulating different realisations of the engine's operation, one can scale the equation of motion into units more physically meaningful to the system. For example, when solving the system's over-damped ODE (i.e. in the absence of stochasticity) within a stationary trap, the colloid's position relaxes to equilibrium at $x_{eq} = \lambda - \frac{m^* g}{\kappa}$, with a relaxation time,

$$\tau_r = \frac{\gamma}{\kappa}\,. \quad (7)$$

Instead, when considering a thermalised colloid, actively absorbing heat from the surrounding fluid, x satisfies Maxwell-Boltzmann statistics. $\langle x \rangle$ is the aforementioned x_{eq}, but now there is an associated standard deviation,

$$\sigma_x = \sqrt{\frac{K_B T}{\kappa}} \,. \tag{8}$$

Scaling times by τ_r and lengths by σ_x yields the nondimensionalised equation of motion,

$$\dot{x}(t) = -\big(x(t) - \lambda(t)\big) - \delta_g + \sqrt{2}\,\xi(t) \,, \tag{9}$$

or in terms of differentials,

$$dx = -\Big[x(t) - \lambda(t) + \delta_g\Big] dt + \sqrt{2\,dt}\, W_t \,. \tag{10}$$

wherein δ_g represents the scaled effective mass, $\delta_g = \frac{m^* g}{\kappa \sigma_x}$. Here we have actually factorised dt from the Wiener increment (previously defined dW), such that W_t is now a random variable distributed according to the standard normal distribution. The chosen units are convenient as now the energy scales in units of $K_B T$.

3.3 Active bath Langevin equation

3.3.1 Active noise models

In addition to the Gaussian noise, generated through heat exchange between the colloid and its surroundings, active noise can also be introduced to the engine by experimentalists. We say this noise is non-equilibrium in nature as it does not abide to a fluctuation-dissipation relation as thermal, equilibrium, noise does. There exists a choice as for the correlation structure possessed by the active noise; two models used within the literature are the the conventional active Ornstein-Uhlenbeck process (AOUP) [5] and the power limited Ornstein-Uhlenbeck process (PLOUP) [6].

When some non-equilibrium noise ζ is added to the system, the SDE for x becomes,

$$dx = \Big[-x(t) + \lambda(t) - \delta_g + \zeta\Big] dt + \sqrt{2\,dt}\, W_t \,. \tag{11}$$

The AOUP and PLOUP ζ models evolve according to the following SDE:

$$d\zeta = -\frac{1}{\tau_c}\,\zeta\, dt + \tau_c^{-n} \sqrt{2 D_{ne}\, dt}\, W_t' \,, \tag{12}$$

Here, $n = 1$ for AOUP and $n = 0.5$ for PLOUP, and W_t' is another random variable acting as a secondary Wiener increment, independent to that describing the thermal noise experienced by the colloid.

A crucial result within stochastic physics is the Wiener-Kninchin theorem. This states that for stochastic processes, which are wide-sense stationary, the process' power spectral density is the Fourier dual of its autocorrelation. The condition of wide sense stationarity is to say that the mean and variance of a process is time invariant. This holds true for the two described models assuming the noise is first allowed to equilbriate. This can be achieved when initialising a simulation's active noise by drawing $\zeta(0)$ from the equilibrium probability density. For the AOUP and PLOUP models,

$$R(\tau) = D_{ne}\tau_c^{(1-2n)}e^{-\frac{\tau}{\tau_c}} \; , \tag{13}$$

$$S(f) = \frac{D_{ne}\tau_c^{2(1-n)}}{1+(2\pi f\tau_c)^2} \; , \tag{14}$$

in which $R(\tau)$ denotes the autocorrelation function for time lag τ and $S(f)$ is the corresponding power spectral density (although missing some Fourier transform normalisation factor). Note that τ_c is called the correlation time as it gives the e-folding time of ζ for both models. In the limit $\tau_c = 0$, the autocorrelation becomes a delta function centered on the origin, and the power spectral density is flat. Hence, we call this the white noise limit of ζ. The names of the two models stem from the fact the total power of AOUP noise is a function of τ_c, whereas for PLOUP noise, the total power is constant with respect to τ_c. Derivations of equations (13) and (14) are shown in appendix A.

The variance in ζ can be recovered through $R(0)$. Doing so reveals why these two models are of interest when asking how differences in active noise correlation structure change the model parameters that optimise free power. The AOUP noise model has a variance inversely proportional to τ_c, and so tends to infinity as correlation time goes to zero. On the other hand, for the PLOUP noise model, the variance in ζ is constant with respect to τ_c. Here, an information engine coupled to AOUP noise was considered, and results from [5] were replicated, to demonstrate successful simulation methods. Then, these results were compared to how correlation time explicitly effects free power output when PLOUP noise is coupled instead, as correlation time no longer impacted fluctuation magnitude.

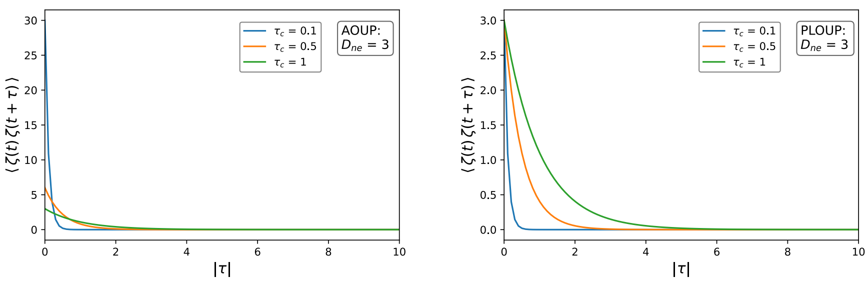

Figure 4: The plots above illustrate the differences between autocorrelation of the AOUP and PLOUP noise models. The intercept, which gives the noise variance, scales as $\frac{1}{\tau_c}$ for AOUP noise, whereas it remains constant for PLOUP noise.

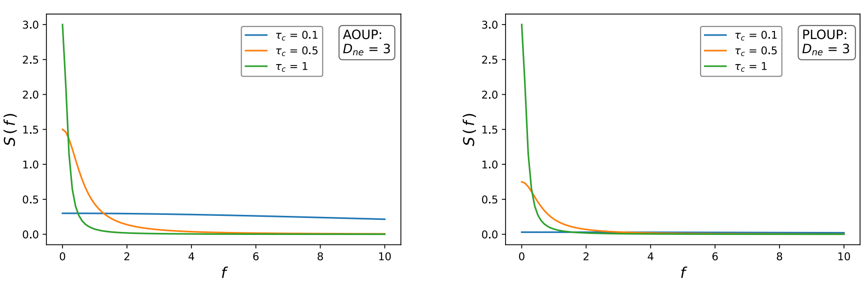

Figure 5: These plots convey how the power spectral densities differ for the two noise models. For the AOUP model, like its autocorrelation, the total power of the noise scales as $\frac{1}{\tau_c}$. On the contrary, the total power for PLOUP noise is independent of its correlation time.

3.4 Feedback protocol

As mentioned in Section 2, the purpose of feedback is to update some work parameter (the trap center here) so as to exploit measurements of the engine's state and produce favourable outcomes. A general form for an information engine's feedback rule, introduced in Lucero et al 2021 [7], is,

$$\Delta\lambda_k = \Theta(x_{k+1} - \lambda_k - \phi)\left[\alpha(x_{k+1} - \lambda_k) + \psi\right]. \tag{15}$$

where $x_{k+1} - \lambda_k$ yields the position of the particle in the trap frame. There are two aspects to such feedback. Firstly, $\Theta(\cdot)$ denotes the Heaviside step function, enforcing the engine's ability to rectify fluctuations up the trap, and ϕ establishes the threshold beyond the trap center in which the particle must cross for the trap to ratchet. If ratcheting will occur, due to the particle fluctuating vertically upwards, α gives the gain as to which the current particle position is scaled, with ψ introducing some constant offset to that product. This linear transformation of the particle position, relative to the trap center, is then the position increment of the trap center. For the information engine simulated here, we choose zero offset and zero threshold,

$$\Delta\lambda_k = \Theta(x_{k+1} - \lambda_k)\alpha(x_{k+1} - \lambda_k)\,. \tag{16}$$

with the latter being chosen such that as many favourable fluctuations as possible are exploited. Maybe experimental realisations of the engine, with some feedback latency, could benefit from a threshold as they can be more confident the particle has not travelled below the trap before the feedback is employed. The frequency of measurements by the feedback controller is taken to be continuous for the similar reason of ratcheting the trap as frequently as possible.

3.5 Engine power types

3.5.1 Free power

Following a ratcheting event, the trap position updates from λ to λ_{k+1} and the change in stored free energy is the increase in equilibrium gravitational potential energy,

$$\Delta F_k = \delta_g(\lambda_{k+1} - \lambda_k) \tag{17}$$

and the corresponding free power is,

$$\dot{F} = \frac{1}{T}\sum_i \Delta F_i\,, \tag{18}$$

where one sums over all ratchet events during the engine's operation, and T is the time over which averaging is performed. This will not equal the full simulation time due to an incorporated burn-in period. This can be simplified to,

$$\dot{F} = \frac{\delta_g}{T}(\lambda_N - \lambda_0)\,, \tag{19}$$

which uses the difference between initial and final gravitational potential energies after N ratchet events.

3.5.2 Trap power

In scaled units, the change in trap potential energy, following a ratcheting event, is,

$$W_k^{trap} = \frac{1}{2}\left[(x_{k+1} - \lambda_{k+1})^2 - (x_{k+1} - \lambda_k)^2\right]\,, \tag{20}$$

and the associated trap power over the engine's operation is given by,

$$\dot{W}^{trap} = \frac{1}{T}\sum_i W_i^{trap} \,. \tag{21}$$

The analysis here follows the ideas seen in [7] in which the engine must store energy by practical means. That is, energy exchanged between the colloidal particle and the noise sources must be channeled into a store of energy which can be later extracted to perform useful work. In this case, gravitational potential energy meets this requirement. If the trap does negative work, i.e. it releases energy as the trap ratchets upwards, it can only be dissipated as heat back into the reservoir, and thus is not practically extractable. Positive trap work corresponds to inputting energy to the system through the trap, but for this to be a pure information engine, there must be no such work. Hence, unless the effect of feedback gain on power is being explicitly explored, the zero trap work feedback scheme is used.

When substituting the expression for λ_{k+1} into the equation for trap work,

$$W_k^{trap} = \frac{1}{2}\alpha(\alpha - 2)(x_{k+1} - \lambda_k)^2 \,, \tag{22}$$

and therefore one can see the trap work is only zero when no feedback is provided at all ($\alpha = 0$) or when the colloidal particle is reflected in the trap center ($\alpha = 2$).

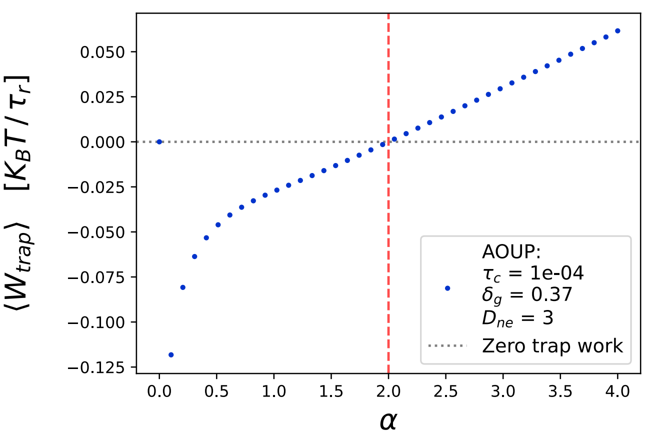

Figure 6: This figure demonstrates how the average work done by the trap varies with the feedback gain. A smaller α means that on average, the shift in trap position per ratchet event is smaller.

4 Numerical Methods for solving SDEs

4.1 Euler-Maruyama update scheme

Instead of solving SDEs analytically, a plethora of finite difference methods can be used, with the aid of a computer, to achieve some desired accuracy of solution. This accuracy must be traded-off with the computational complexity, and hence length of time, required to extract such approximate solutions. Consider again the nondimensionalised SDE for a colloid in a Gaussian bath, seen in equation (10). The simplest method for evaluating a step in x is to approximate the differentials with finite intervals,

1. $\Delta x = -\Big[x_n - \lambda_n + \delta_g\Big]\Delta t + \sqrt{2\,\Delta t}\,W_t$
2. $x_{n+1} = x_n + \Delta x$

This is the Euler-Maruyama (EM) method. Here, $n \in \mathbb{Z}$, $0 \leq n \leq N$ and $N = \frac{T}{\Delta t}$, where T is the duration of the simulated x trajectory. Note, that Δt is a constant of the simulation which is sufficiently small to avoid significant discretisation error, but not incessantly small so as to increase computational complexity unnecessarily.

There does exist an alternate numerical method for solving SDEs known as the Milstein's update scheme, which can show higher orders of strong convergence. However, in the case of additive noise (no x dependence), as seen in the OU processes discussed thus far, Milstein's method reduces to the EM method.

4.2 Heun's update scheme

Unlike the Milstein method, one update scheme which can be used to increase the strong convergence of additive noise SDEs is the Heun's method [8]. It does so by functioning as a predictor-corrector method, minimising the likelihood of solutions suffering from instability. The Heun's method for equation (12) is implemented as shown below:

1. $\Delta\zeta = -\frac{1}{\tau_c}\,\zeta_n\,\Delta t + \tau_c^{-n}\sqrt{2D_{ne}\,\Delta t}\,W_t'$,
2. $\hat{\zeta}_{n+1} = \zeta_n + \Delta\zeta$,
3. $\zeta_{n+1} = \zeta_n - \frac{1}{2\tau_c}\,(\zeta_n + \hat{\zeta}_{n+1})\,\Delta t + \tau_c^{-n}\sqrt{2D_{ne}\,\Delta t}\,W_t'$

The estimator of ζ_{n+1} utilised is its value calculated via the EM method.

4.3 Effective simulation

When using computers to simulate trajectories of the information engine, the particle's position will demonstrate some transient response to the engine, prior to settling into steady state ratcheting. This part of the trajectory will not conform to theoretical expectations and should therefore be discarded. This is called a burn-in period and, for the simulations performed here, a burn-in period equal to 40% of the operational time was used. In addition to this, in an attempt to reduce the length of such transient behaviour, the particle's initial position was drawn from its distribution for an equilibriated particle in a stationary trap. This was found by writing a 2D vector SDE, containing both the evolution of x and ζ, and the system's Fokker-Planck equation was then set to zero (as done in [5]). This corresponds to the probability distribution of positions reaching stationarity. This distribution takes the form,

$$x \sim N\Big(x_{eq},\, 1 + \frac{D_{ne}\tau_c^{2(1-n)}}{1+\tau_c}\Big)\,, \tag{23}$$

with n differentiating the distributions for an engine coupled to AOUP or PLOUP active noise.

Given that OU processes are Markovian, the probability of subsequent evolutions of x depends solely upon its current value. The physical intuition behind such motion is the fact particles are devoid of momentum in the over-damped regime. Therefore, the length of the simulation should be inconsequential, assuming the particle has been allowed sufficient time to first relax into its steady state, as averaging over many shorter trajectories functions equivalently when sampling Markov processes. Simulating the engine over smaller time periods would give a smaller discretisation error for the same number of time steps. That being said, the mean power statistics may be weaker for shorter simulations, and thus one would need to average over more trajectories to achieve the same error on the mean. Taking both these factors into account, a simulation time of 25 was chosen (25 τ_r in physical units).

For the results shown in this review, each calculation of mean power was associated with an ensemble of 1000 sample trajectories. The simulated trajectories of active noise used the Heun's method as it allows greater strong convergence than that seen by the EM method. On the other hand, the EM method was still implemented to simulate the trajectories for the colloidal particle position; this was because the discrete nature of a ratchet event means the predictor-corrector method may not accurately describe the x drift term. To quantify the shortcomings of using numerical methods, bootstrapping was performed on these trajectory ensembles to find the standard errors of the mean powers. The Δt used for its insignificant discretisation error was 10^{-4}, which in physical units corresponds to a ten thousandth of a relaxation time for the colloidal particle.

Note that the code used for these simulations is linked in Appendix B.

5 Results

5.1 Free powers as a function of δ_g

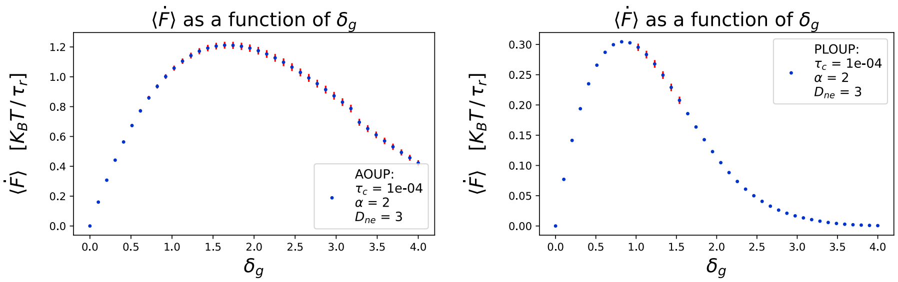

Figure 7: The above plots show how the mean free power output of the information engine varies as a function of the scaled effective mass, δ_g, for both the AOUP and PLOUP noise models in their white noise limits.

For the AOUP noise model, the free power, for a given noise strength and correlation time, is maximised at an intermediary δ_g. This was also shown in [5], however here it has been shown that the PLOUP noise model also exhibits similar behaviour. The intuition behind this involves a trade-off between two approaches towards increasing free power output. The first is to use a small δ_g; given that δ_g is the equilibrium mean separation of the particle and the trap center, it having a small value suggests that the particle needs to drift less from equilibrium to induce a ratchet event. More frequent ratchet events equates to a higher free power. Instead, if δ_g is large, although ratcheting may be rarer, it results in a greater store of gravitational potential energy. The balance struck between rapid and substantial storage of free energy creates the skewed bell curves seen in figure 7.

Note that despite D_{ne} and τ_c being equal for two data sets, there exists a discrepancy between the noise models. In the white noise limit, the variance of PLOUP ζ is 3, whereas it equals 30,000 in the AOUP case. This means a particle interacting with AOUP noise need not worry so much about being close to the trap center, as in general the magnitude of fluctuations are much larger. Therefore, greater prioritisation should be given to a larger δ_g to store more free energy per ratchet event. As correlation time decreases, and variance increases, the peak free power is higher and at a higher δ_g.

5.2 Free powers as a function of τ_c

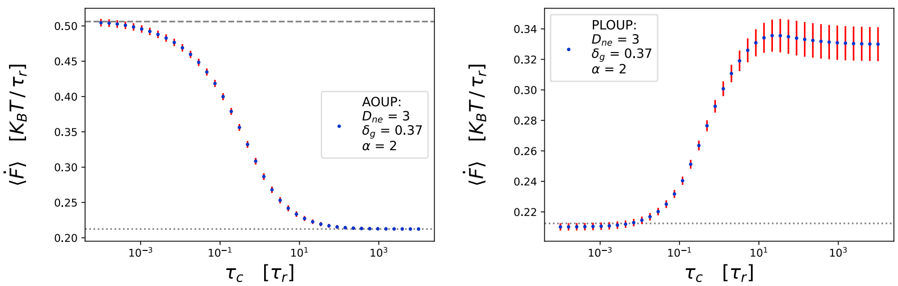

Figure 8: Shown above is the free power output of the engine, as a function of noise correlation time, for both the AOUP and PLOUP noise models.

It is clear that the dependency of free power on correlation time varies notably between the two noise models. The results within Saha et al 2023 [5], which used AOUP noise, have been reproduced here, with τ_c being the reciprocal of the parameter f_{ne} used there. As they discussed, the variance in active noise is greater for low correlation times, resulting in generally larger particle fluctuations and more frequent ratcheting. It is more beneficial for the Gaussian-active bath composite to behave like a Gaussian bath of higher effective temperature than it is for the engine to explicitly exploit correlations in the AOUP noise. For high τ_c, the variance in ζ tends to zero and thus the free power output tends to that seen when there is exclusively thermal noise. The white-noise limit of the active noise was derived in [5], with the original result for a Gaussian bath being derived in [4]. They did so with the theory of mean first passage times and that result can be modified to apply here given the Gaussian-active bath composite is taken in its white-noise limit.

On the other hand, since the variance in ζ is constant with respect to τ_c for PLOUP noise, an effective Gaussian bath cannot be established. Instead, the engine exhibits a preference towards more strongly correlated active noise. The center of the curve is visibly of order τ_r in physical units. For correlation times shorter than the characteristic relaxation time of the colloidal particle, it cannot respond quickly enough for the fluctuation to be fully exploited. For high correlation times, downwards ζ values are not detrimental to engine performance as the trap prevents the particle drifting too far downwards; therefore, its always reasonably close to a ratchet event despite strong correlation downwards. However, if the strong correlation in ζ is upwards, the trap continually ratchets upwards with each storing free energy. The limited disadvantage of downwards correlation and great advantage of up correlation seems to justify why higher correlation times are beneficial. Within the PLOUP plot, the free power output peaks and then decreases before asymptoting to some high τ_c limit. This peak is suspected to be an artefact of ineffective simulation of the engine, as one wouldn't expect anything but a monotonic curve here. A longer simulation time per sample is needed to capture the benefits of larger correlation times, and to allow for the engine to relax into its steady state. This flaw in simulation is discussed in more detail later.

5.3 Free powers as a function of D_{ne}

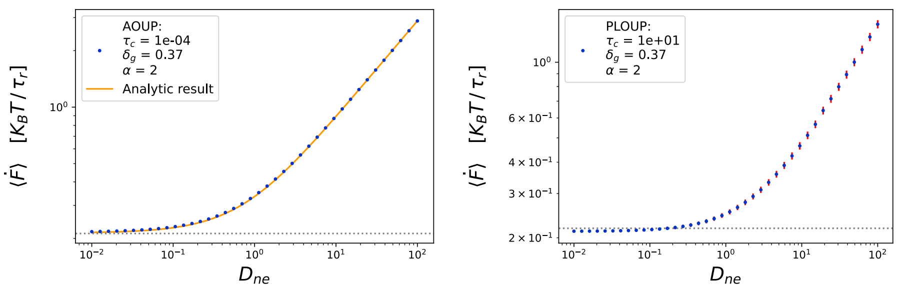

Figure 9: Shown above is the free power output of the engine, as a function of noise strength, for both the AOUP and PLOUP noise models.

Figure 9 shows that, for both noise models, increasing the noise strength increases the free power output. The analytic curve added to the AOUP plot is the white noise limit of the Gaussian-active bath composite, as mentioned in 5.1. These curves begin growing away from the asymptotic, Gaussian bath, limit at different D_{ne} values and this is due to differences in τ_c dependence between the experienced forces from these active noise models. Here the appeal of active baths becomes evermore evident; the free power output can be increased indefinitely without the need to increase the temperature of the engine, which could begin to negatively impact its operation.

6 Simulation improvements and future research areas

The primary improvement to be made in additional simulations, stemming from code used in this project, is to use a super trajectory. This could be partitioned into 1000 samples, as opposed to using the current samples which are 1000 separate trajectories. This is beneficial as each simulation has some burn-in period required for the engine to relax into its steady state. The PLOUP results fail due to a burn-in period which is far too short for long correlation times, in which the system still "remembers" the system initialisation. If one wants a burn-in period at least 10 times the maximum considered correlation time, it wastes computational time to relax the system 1000 times instead of once, at the start of a super trajectory. For n sample trajectories, a super trajectory $n+1$ times the desired sample time should be ran with the first "sample" discarded as the burn-in. Then, the data could be gathered again and the PLOUP results improved at high τ_c.

As for some extensions to these simulations, it may be worthwhile exploring if the implemented feedback protocol can be modified to make more explicit use of any correlations. One approach to this, as suggested by my project Mentor Johan du Buisson, is to include an additional Heaviside step function factor containing the difference between the current and immediately previous particle position. This captures a sort of velocity of the particle, indicating the direction of the noise correlations. Perhaps if the information engine is not lossless, unlike that assumed here, such conditions can increase the free power output. There may be a means of parameterising the weight given to this instantaneous velocity factor through τ_c; for example, the event of a favourable upwards velocity is meaningless in the white noise limit and so should not factor into whether ratcheting occurs, hence the need for some appropriate weighting.

Moreover, the act of measuring the particle's position and resetting the memory of the feedback controller involves some energetic cost. This could be calculated for this engine [9], and a net power output could be plotted also. Positive average free power output does not guarantee the information engine will be useful, as the feedback cost may be high, and the net power negative.

7 Conclusion

To conclude, for the AOUP noise model, in which fluctuation variance decreases with stronger correlations, it is in fact disadvantageous for the noise to be correlated. The free power saturates in the white noise limit, wherein the active bath mimics the thermal, Gaussian, bath. On the contrary, for PLOUP noise, with its τ_c independent fluctuation variance, these results suggest an inherent benefit to strongly correlated noise when optimising the free power output of the information engine. A key improvement to the simulation procedure is to replace the current trajectory ensemble with samples from a super trajectory, requiring a single burn-in period. A next step towards probing the utility of an information engine coupled to PLOUP noise would be to include feedback costs, and calculate a net power output.

Appendices

A Active noise calculations

The general SDE used to describe the AOUP and PLOUP noise models is,

$$d\zeta = -\frac{1}{\tau_c}\,\zeta\,dt + \tau_c^{-n}\sqrt{2D_{ne}}\,dW\,, \tag{24}$$

as seen in equation (10), except with a non-factorised Wiener increment, and here the prime notation to distinguish thermal and active noise increments has been dropped. One can make the substitution $z = \zeta\, e^{\frac{t}{\tau_c}}$, as used by Jacobs in Stochastic Processes for Physicists [10], to simplify the SDEs solution:

$$\begin{aligned} dz &= z(\zeta + d\zeta, t + dt) - z(\zeta, t) \\ &= (\zeta + d\zeta)\, e^{\frac{t+dt}{\tau_c}} - \zeta\, e^{\frac{t}{\tau_c}}\,, \end{aligned}$$

and using the fact that, in the infinitesimal limit, $e^{\frac{dt}{\tau_c}} = 1 + \frac{dt}{\tau_c}$,

$$\begin{aligned} dz &= (\zeta + d\zeta)\, e^{\frac{t}{\tau_c}}(1 + \frac{dt}{\tau_c}) - \zeta\, e^{\frac{t}{\tau_c}}\,, \\ &= \frac{1}{\tau_c}\zeta e^{\frac{t}{\tau_c}}\, dt + d\zeta\, e^{\frac{t}{\tau_c}}\,, \\ &= \frac{z}{\tau_c} dt + d\zeta\, e^{\frac{t}{\tau_c}}\,, \end{aligned}$$

where we have used the fact the product $dt\, d\zeta$ is quadratic in small quantities. Substituting equation (24) into $d\zeta$ above yields,

$$dz = \tau_c^{-n}\sqrt{2D_{ne}}\, e^{\frac{t}{\tau_c}}\, dW\,,$$

which can be integrated for,

$$\begin{aligned} z(t) &= z_0 + \tau_c^{-n}\sqrt{2D_{ne}} \int_0^t e^{\frac{s}{\tau_c}}\, dW(s), \\ \zeta(t) &= \zeta_0\, e^{\frac{-t}{\tau_c}} + \tau_c^{-n}\sqrt{2D_{ne}} \int_0^t e^{\frac{(s-t)}{\tau_c}}\, dW(s)\,. \end{aligned}$$

Note $\langle\zeta\rangle$ is zero as the mean of the Wiener increment itself is zero. One can find the corresponding autocorrelation of this noise for time lag τ via,

$$R(\tau) = \langle\zeta(t)\zeta(t+\tau)\rangle = \langle\zeta(t)\rangle\, e^{\frac{-t}{\tau_c}} + 2D_{ne}\tau_c^{-2n}\Big\langle \int_0^t e^{\frac{(s-t)}{\tau_c}}\, dW(s) \int_0^{t+\tau} e^{\frac{(s'-t-\tau)}{\tau_c}}\, dW(s')\Big\rangle\,,$$

where we have used the fact the mixed products are linear in an averaged stochastic integral, which equals zero, and s' is just another dummy variable. The first term is zero as we now assume ζ has evolved for long enough to reach its stationary distribution. Focusing on the last term, and decomposing the latter expectation into two time intervals,

$$R(\tau) = 2D_{ne}\tau_c^{-2n}\Big[\Big\langle \int_0^t \int_0^t e^{\frac{(s+s'-2t-\tau)}{\tau_c}}\, dW(s)\, dW(s')\Big\rangle + \Big\langle \int_0^t e^{\frac{(s-t)}{\tau_c}}\, dW(s) \int_t^{\tau} e^{\frac{(s'-\tau)}{\tau_c}}\, dW(s')\Big\rangle\Big]\,.$$

Now the last term is a product of two independent pieces of the noise's evolution, hence the average of their product is zero, and only the first term remaining. This term can be rewritten as,

$$R(\tau) = 2D_{ne}\tau_c^{-2n}\, e^{-\frac{(2t+\tau)}{\tau_c}} \int_0^t \int_0^t e^{\frac{(s+s')}{\tau_c}} \langle dW(s)\, dW(s')\rangle$$

and as mentioned in the introduction to the Wiener increment, its autocorrelation is delta distributed. Therefore,

$$\begin{aligned} R(\tau) &= 2D_{ne}\tau_c^{-2n}\, e^{-\frac{(2t+\tau)}{\tau_c}} \int_0^t e^{\frac{2s}{\tau_c}}\, ds \\ &= (1+e^{-\frac{2t}{\tau_c}})D_{ne}\tau_c^{(1-2n)}\, e^{-\frac{\tau}{\tau_c}}\,. \end{aligned}$$

Clearly, in the limit as $t \to \infty$, i.e. ζ approaches its stationary distribution, the autocorrelation is,

$$R(\tau) = D_{ne}\tau_c^{(1-2n)}\, e^{-\frac{\tau}{\tau_c}}\,.$$

Evaluating the autocorrelation at a time lag of zero yields the variance,

$$Var(\zeta) = D_{ne}\, \tau_c^{(1-2n)}\,.$$

Given that the mean and variance of ζ have been shown as time invariant, the Wiener-Kninchin theorem applies. Taking the Fourier transform (excluding a normalisation constant) shows the power spectral density for exponentially correlated noise is Lorentzian:

$$\begin{aligned} S(f) &= D_{ne}\tau_c^{(1-2n)} \int_{-\infty}^{\infty} e^{-\frac{\tau}{\tau_c}}\, e^{-2\pi i f\tau}\, d\tau. \\ &= \frac{D_{ne}\tau_c^{2(1-n)}}{1+(2\pi f\tau_c)^2}\,. \end{aligned}$$

B Simulation repository

The code used when simulating this information engine can be found at:

https://github.com/LewisDean22/sivak_group_summer_project.git

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