On the Scalability of Evolution Strategies in the Optimization of Dynamic Molecular Alignment

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ABSTRACT

We consider the numerical optimization of dynamic molecular alignment by shaped femtosecond pulses, and study the scalability of the electric field subject to optimization by Evolution Strategies. The trade-off between fine-tuning of the electric field versus the *evolutionary* optimization feasibility is investigated.

Categories and Subject Descriptors

I.2.8 [**Computing Methodologies**]: ARTIFICIAL INTELLIGENCE—*Problem Solving, Control Methods, and Search*

General Terms

Algorithms, Experimentation, Performance

Keywords

Scalability, Evolution Strategies, Laser Pulse Shaping

1. INTRODUCTION

The goal of our research is to optimize the *alignment* of an ensemble of diatomic molecules after the interaction with a shaped laser pulse. Here we consider the optimization of dynamic molecular alignment by a specific *derandomized* Evolution Strategy [1]. The task is defined as the calibration of the electric field, based on a low-dimensional parameterization. An important issue for this physics application is the dimensional scalability, i.e., increasing the number of variables, aiming to provide a more appropriate, fine-grained modeling approach for the problem. We question whether there exists an optimal parameterization for this problem, which allows fine-tuning of the laser pulse shaping process, but is also feasible from the optimization perspective. The role of the experimental feedback in the self-learning loop is played here by a numerical simulation [2].

The time-dependent profile of the laser pulse is described by: $E(t) = \int_{-\infty}^{\infty} A(\omega)\exp(i\phi(\omega))\exp(i\omega t)\ d\omega$. $A(\omega)$ is a Gaussian window function describing the contribution of different frequencies to the pulse and $\phi(\omega)$, the *phase function*, equips these frequencies, which are equally distributed across the spectrum of the pulse, with different complex phases. $\phi(\omega)$ is interpolated at n frequencies $\{\omega_i\}_{i=1}^{n}$; the n values $\{\phi(\omega_i)\}_{i=1}^{n}$ are the decision parameters to be optimized. The alignment's success-rate is defined as the expectation value of the *cosine-squared* of the angle of the molecular axis with respect to the laser polarization axis.

From the numerical-technical aspect, one should keep in mind that these n decision parameters are eventually *interpolated* into $N^* = 16,384$ function values which are transformed into the electric field in the so-called *Schrödinger simulation*.

2. RESULTS AND DISCUSSION

When subject to $10,000$ function evaluations, the best results were obtained for the low-dimensional parameterization, $n = \{80, 100, 120, 140\}$, forming a decreasing curve of performance as the dimensionality increases. Successful learning of the decision parameters was typically observed after $\approx 5,000$ function evaluations, and was not achieved for the high-dimensional cases. When more function evaluations were granted, the optimization routine succeeded in locating a high-quality solution even for a parameterization of $n = 1,000$ decision parameters.

From the algorithmic perspective, we may conclude that the derandomized ES variant in use was capable of optimizing a large number of decision parameters. However, from the *physics* perspective, such a high-resolution parameterization does not seem to pay-off, as far as the cosine-squared alignment is concerned, and there seems to be no justification for allowing more phase function values to be optimized.

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3. REFERENCES

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