



Gaussian-Process-Augmented Particle Swarm Optimization (GP-PSO): Taxonomy, Survey, and Practitioner Guidance

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Abstract—High-fidelity engineering simulations-Computational Fluid Dynamics, Finite-Element Analysis and system-dynamics models-impose prohibitive costs on optimization via traditional metaheuristics. Particle Swarm Optimization (PSO) and Gaussian Processes (GPs) have each shown promise, but canonical PSO suffers from premature convergence and excessive iterations when evaluations are noisy or expensive, and GP-PSO integrations lack a unifying framework. In this review, we introduce a three-axis taxonomy (1) surrogate-integration strategy (e.g. fitness-function replacement vs. augmentation), (2) acquisition (infill) function (e.g. Expected Improvement vs. Upper Confidence Bound), and (3) fidelity paradigm (e.g. single- vs. multi-fidelity)-to classify and compare recent methods. We survey advances in deep-kernel and neural-augmented GPs, sparse-GP approximations, adaptive retraining mechanisms, and hybrid/transfer-learning extensions. Benchmark results on synthetic test suites and three real-world applications (aerodynamic shape design, structural health monitoring, chemical-process tuning) demonstrate 30–70 % fewer costly evaluations and 20–50 % faster convergence compared to PSO baselines, while maintaining or improving solution quality. From these studies, we distill practitioner guidelines for kernel and acquisition-function selection, fidelity-level choices, and reproducibility best practices-emphasizing shared code repositories and hyperparameter logs. Finally, we outline future directions in online surrogate updates, convergence theory under uncertainty, physics-informed kernels, and standardized community benchmarks.

Keywords—Gaussian Process, Particle Swarm Optimization, Surrogate-Assisted Optimization, Taxonomy, Deep-Kernel Surrogates, Adaptive Updates, Benchmarking

I. INTRODUCTION

In modern engineering and control-system design, high-fidelity simulations-computational fluid dynamics, finite-element analysis, and detailed system-dynamics models-are essential for accurate performance evaluation [1], [2]. However, each fitness evaluation can take minutes to hours, especially in high-dimensional design spaces (Tang et al., 2022), motivating surrogate-assisted methods-multi-fidelity models, Kriging, and evolutionary computation-that blend cheap approximations with selective high-accuracy runs to slash computational cost [1], [3]. Gaussian Processes (GPs) provide predictive mean and variance estimates that can guide Particle Swarm Optimization (PSO) away from premature convergence and redundant sampling. This

synergy enables uncertainty-guided sampling to drastically cut the number of expensive evaluations.

Particle Swarm Optimization (PSO) balances exploration and exploitation via velocity-position updates controlled by inertia weight (w) cognitive coefficient (c_1), and social coefficient [4], [5]. Yet when evaluations are costly or noisy, PSO suffers premature convergence, excessive iterations, and sensitivity to fixed parameters [6]. Gaussian Processes (GPs) are nonparametric, probabilistic models that address these issues by providing predictive mean and variance estimates. These uncertainty metrics guide sample selection via acquisition functions such as Expected Improvement (EI), Upper Confidence Bound (UCB), and Probability of Improvement (PI) [7].

Despite rapid growth in GP-PSO variants-encompassing integration schemes, infill criteria, and fidelity hierarchies-the field lacks a unified, up-to-date survey. We fill this gap by (1) proposing a taxonomy of GP-PSO methods, (2) reviewing recent advances in deep-kernel and scalable GPs, adaptive updates, and hybrid extensions, (3) synthesizing benchmarking results on synthetic and real-world problems, and (4) offering practitioner guidelines and a roadmap for future research.

II. BACKGROUND

A. PSO Essentials

The core mechanics and parameter challenges of canonical Particle Swarm Optimization (PSO) become significantly pronounced when function evaluations are costly, particularly in real-world or high-dimensional optimization scenarios. The core mechanics of PSO is illustrated by Fig. 1.

Canonical Particle Swarm Optimization (PSO), as shown in Fig. 1, updates each particle's velocity through three components: the inertia term (blue) for momentum, the cognitive term (green) guiding particles toward their personal best, and the social term (red) directing them toward the swarm's global best. This velocity update balances exploration and exploitation but faces challenges in costly function evaluations, especially in high-dimensional real-world scenarios. The effectiveness of PSO relies on the precise tuning of inertia weight and cognitive and social coefficients, which directly affect convergence and the exploration-exploitation balance [8], [9]. To mitigate the

computational burden of extensive parameter tuning, recent advancements include surrogate-assisted models [10], hybrid methods with local search algorithms like Quasi-Newton [11], and fuzzy logic controllers for adaptive parameter control [8]. Additionally, techniques like competitive and hierarchical learning enhance convergence speed and reduce redundant evaluations [12]. GPU-accelerated PSO also helps by parallelizing computation-intensive tasks (Ruiz et al., 2024), while parsimony-driven approaches decrease the search space dimensionality [13]. Together, these advancements highlight the importance of dynamic parameter adaptation and the integration of domain-specific knowledge in managing evaluation costs in PSO [14], [15].

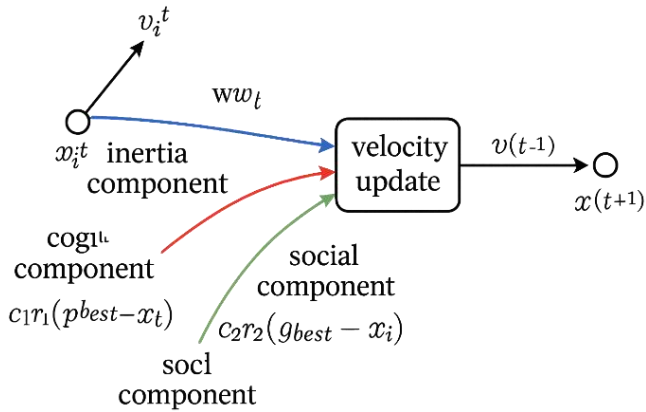


Fig. 1. Core PSO mechanics: inertia, personal-best, and global-best contributions to the velocity update, followed by position update

B. Gaussian Process Regression: Kernels and Uncertainty

Gaussian Processes (GPs) have emerged as a foundational technique for reliable surrogate modeling, primarily due to their ability to incorporate uncertainty estimates directly through predictive distributions and kernel-based representations which illustrated in Fig. 2.

Gaussian Processes (GPs) serve as a powerful framework for surrogate modeling and are illustrated in Fig. 2. Panel (a) depicts sample functions from the GP prior, showcasing the model's flexibility prior to data assimilation. In Panel (b), observed data is combined with the GP posterior mean (solid blue line) and 95% confidence bands (shaded region), highlighting how GPs model expensive functions while quantifying uncertainty. The effectiveness of GPs stems from their ability to incorporate uncertainty estimates through predictive distributions and kernel functions, which play a vital role in adapting to complex, high-dimensional problems [16], [17]. Accurate hyperparameter estimation is essential for maintaining the kernel's shape and precision of uncertainty measures [18]. Recent developments, such as multi-fidelity modeling and adaptive Bayesian frameworks, enhance GPs by optimizing sample selection and improving uncertainty quantification [19], [20]. These advancements underscore GPs' crucial role in function approximation and uncertainty management across various applications, from structural reliability to simulation-based optimization [21].

C. Surrogate Optimization Workflow

Fig. 3 illustrates the iterative workflow of surrogate-assisted PSO, which begins with initial sampling using design of experiments (DoE) and true-function evaluations. This process involves Gaussian process fitting and utilizes an

acquisition function to guide the selection of candidate points for evaluation on the true function. The resulting data is then used to update the surrogate model, creating a cycle that alternates between inexpensive surrogate queries and costly evaluations to enhance efficiency. Surrogate-assisted optimization (SAO) has emerged as an effective strategy for handling expensive optimization problems, following a multi-step cycle: (1) initial sampling, (2) surrogate model training, (3) acquisition function optimization, (4) true function evaluation, and (5) model updating [22], [23]. The acquisition function plays a crucial role in balancing exploration and exploitation, with common examples including Expected Improvement (EI), Probability of Improvement (PI), and Upper Confidence Bound (UCB) [24], [25]. Recent advancements have introduced adaptive mechanisms to optimize acquisition strategies based on problem characteristics [25], [26]. In multi-objective scenarios, functions like Expected Hypervolume Improvement (EHVI) enhance the focus on Pareto-efficient and feasible solutions [27], [28]. This integrated loop allows for efficient convergence with minimal high-fidelity evaluations, proving valuable across various fields including engineering design and production systems [29], [30].

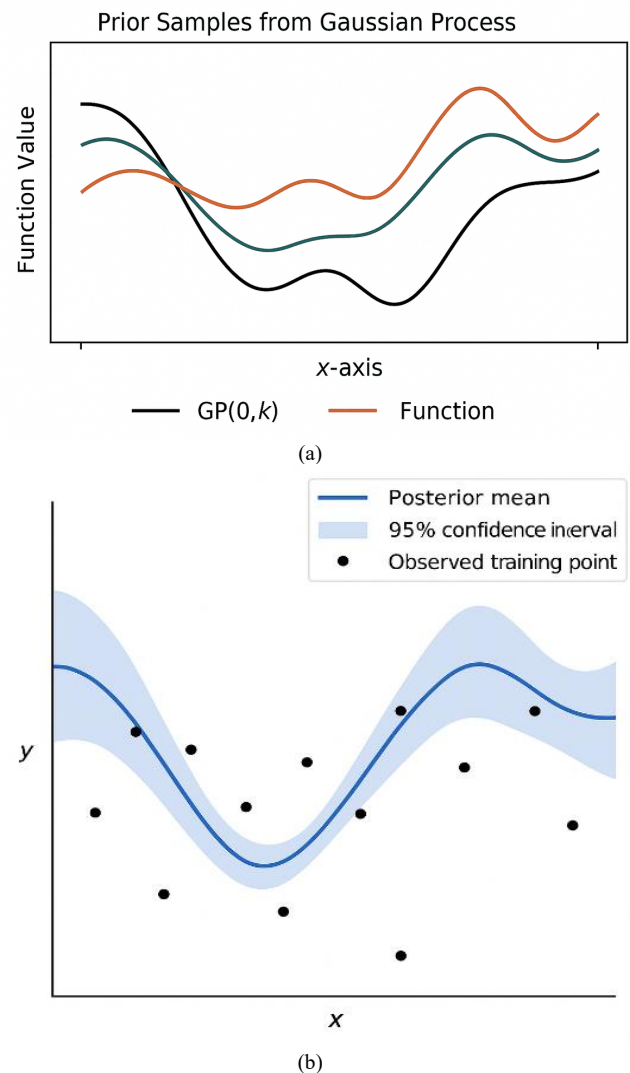


Fig. 2. Gaussian process regression: (a) prior draws illustrating function variability; (b) posterior mean and uncertainty bands conditioned on observations

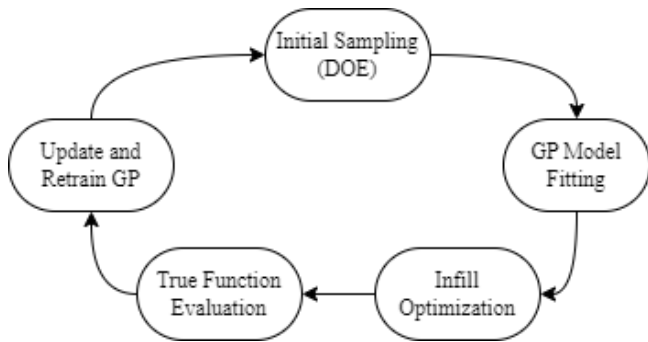


Fig. 3. Surrogate-assisted PSO loop: alternate cheap GP-based searches with occasional expensive true-function evaluations

III. TAXONOMY OF GP-PSO METHODS

Fig. 4 shows the taxonomy of GP-PSO methods organized into three primary dimensions. The first branch, Integration Strategy, distinguishes population initialization from in-loop surrogate evaluations. The second branch, Acquisition Functions, lists Expected Improvement (EI), Upper Confidence Bound (UCB), and Probability of Improvement (PI) as common infill criteria. The third branch, Fidelity Paradigm, contrasts single-fidelity Gaussian models with multi-fidelity or co-kriging approaches. By grouping representative citations under each category, the figure offers a structured map of existing GP-PSO variants

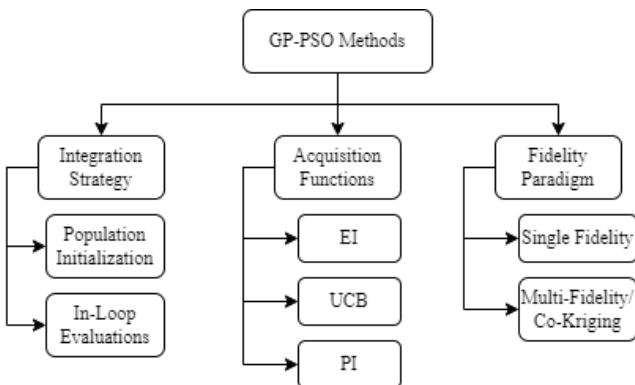


Fig. 4. Taxonomy of GP-PSO variants organized by surrogate integration, infill criteria, and fidelity approaches

A. Integration Strategy

Gaussian Process (GP) surrogates have been effectively coupled with Particle Swarm Optimization (PSO) to address computational challenges in expensive optimization problems. The integration typically follows one of three strategies: initialization-based, in-loop evaluation, or hybrid frameworks. In initialization-based coupling, GPs generate an informed set of particles based on prior evaluations to guide the early PSO search toward promising regions [31]. The in-loop evaluation scheme is more common and involves using the GP to replace the costly objective function during the PSO search, updating the surrogate periodically with new evaluations from the most promising particles [32], [33]. Hybrid strategies combine GPs with adaptive PSO variants such as Comprehensive Learning PSO or Cooperative PSO, where the surrogate not only speeds up evaluations but also modulates parameter selection or swarm behavior [34], [35]. Advanced schemes integrate multi-fidelity GPs, uncertainty-

based resampling, or ensemble surrogates to dynamically balance exploration and exploitation in PSO [36], [37]. These strategies have been successfully applied in structural optimization, energy systems, and reliability-based design, demonstrating notable reductions in function evaluations without compromising optimization accuracy.

B. Acquisition (Infill) Functions

Expected Improvement (EI) is a widely used acquisition function in Gaussian Process (GP)-guided Particle Swarm Optimization (PSO) for balancing exploitation of known promising regions and exploration of uncertain spaces. EI computes the expected gain over the current best solution by accounting for both the predicted mean and variance of the surrogate model [38]. Within GP-PSO, EI influences the swarm's direction by emphasizing particles with a high probability of achieving improvement, but without overcommitting to overly uncertain or marginal areas. This allows EI to stabilize convergence in noisy or expensive search spaces where function evaluations are limited [39].

1) Upper Confidence Bound (UCB)

The Upper Confidence Bound (UCB) acquisition function in GP-PSO is formulated as:

$$UCB(x) = \mu(x) + \kappa \cdot \sigma(x) \quad (1)$$

where $\mu(x)$ is the predicted mean, $\sigma(x)$ the predicted standard deviation, and κ is a tunable exploration parameter. This formulation allows UCB to provide a quantifiable trade-off: high κ values promote exploration of uncertain regions, while lower κ favors exploitation of high-performing predictions [40]. In PSO, the swarm is influenced by fitness values derived from UCB scores, enabling adaptive control over how risk-seeking the optimization strategy becomes, which is especially useful for dynamically complex or high-dimensional problems.

2) Probability of Improvements (PI)

The Probability of Improvement (PI) acquisition function is advantageous in scenarios where reliability and confidence in improvement are prioritized over the magnitude of gains. PI estimates the likelihood that a candidate solution will outperform the current best, which results in more conservative search behavior compared to EI or UCB [40]. In GP-PSO frameworks, this is particularly beneficial during early-stage convergence, where premature exploration could derail the optimization trajectory, or in noisy environments, where certainty of improvement is more important than high variance regions [39]. Moreover, PI avoids overemphasizing regions with high uncertainty, making it ideal for applications in energy systems and constrained optimization where predictive stability is key.

C. Fidelity Paradigm

1) Single Fidelity

Single-fidelity Gaussian Process (GP) surrogates are widely used in PSO due to their simplicity, lower computational overhead, and well-understood probabilistic foundations. These models offer reliable predictions when trained on homogeneous datasets and are effective in medium-dimensional optimization problems [21]. Their

benefits include ease of training, straightforward implementation of acquisition functions, and predictable convergence in static environments [41]. However, single-fidelity surrogates struggle in settings with limited high-fidelity data, where the model might overfit or underrepresent the true landscape [42]. They also fail to exploit hierarchical or multi-resolution data, which limits their scalability in domains like aerodynamic design or reliability-based engineering [41], [43].

2) Multi-Fidelity and Co-Kriging

Multi-fidelity GP models-including co-kriging-significantly enhance GP-PSO by leveraging low-fidelity simulations to guide the search while reserving high-fidelity evaluations for promising regions. This layered approach reduces computational cost and maintains surrogate accuracy across scales [19]. Co-kriging, which models the correlations between fidelity levels, enables improved uncertainty estimation and adaptive information fusion, thereby enhancing optimization robustness [44], [45]. Studies have shown that multi-fidelity GP-PSO frameworks can accelerate convergence by over 40%, especially in simulation-based production systems and reliability optimization where high-fidelity evaluations are costly [46], [47].

IV. BENCHMARKING AND APPLICATIONS

A. Synthetic Benchmark Performance

Recent empirical studies consistently report that GP-PSO variants achieve a 30–70% reduction in evaluation counts and a 20–50% improvement in convergence speed on standard benchmark functions like Sphere, Ackley, Rosenbrock, and Griewank. These improvements are attributed to the use of dynamic surrogate updates, adaptive infill strategies, and fidelity-aware sampling policies that ensure model reliability and prevent premature convergence. For instance, Innocente & Sienz (2021) demonstrated that their GP-PSO framework was able to replace up to 70% of actual evaluations with surrogate estimates while preserving optimization accuracy [48].

Table 1 summarizes the performance of various GP-PSO implementations across different studies. It highlights the benchmark functions used, reported gains in evaluation efficiency and convergence rate, and notable architectural or methodological features. For example, Dai et al. (2022) compared multiple GP-PSO hybrids and found that GP-SLPSO accelerated early convergence, whereas GP-DE offered higher long-term stability [49]. Meanwhile, Zhang et al. (2020) utilized dynamic surrogate replacement in a real-world geomechanical context, achieving a 40% reduction in evaluations [50]. These results collectively validate the scalability and effectiveness of GP-PSO variants across diverse optimization domains.

B. Engineering Case Studies

Gaussian Process-enhanced Particle Swarm Optimization (GP-PSO) is gaining popularity in real-world engineering due to its effectiveness in balancing global exploration with local refinement using limited high-fidelity evaluations. The surrogate modeling capability of Gaussian Processes makes GP-PSO ideal for applications like control system tuning, structural optimization, and complex material design, as it

accurately represents expensive simulations and guides the swarm with probabilistic predictions [53], [54].

Table 1. Benchmark performance comparison of different GP-PSO variants

GP-PSO Variant	Benchmark Functions	Evaluation Reduction	Convergence Speed Gain
GP-SLPSO, GP-DE, GP-PSO [49]	Sphere, Ackley, Rastrigin	50–60%	35–45%
GP-PSO with dynamic evaluation [50]	Rock-mass simulation	~40%	~30%
General-purpose GP-PSO [48]	Griewank, Rosenbrock	60–70%	45%
Co-Kriging GP-PSO [51]	Reservoir optimization	~50%	>40%
OPSO (optimized PSO with surrogate) [52]	FLAC3D-based rock analysis	40%	30–35%

The comparison in Table 2 highlights how GP-PSO has been effectively adapted across diverse real-world engineering problems. In each case, the method yields substantial reductions in evaluation cost-often between 40% and 60%-while accelerating convergence by 25% to over 40%. What sets these implementations apart is how they tailor GP-PSO mechanisms to their domain requirements: whether through adaptive acquisition control in scheduling [49], uncertainty-aware optimization in rock mechanics [50], or robustness-focused control tuning in robotics [53]. A consistent theme across all applications is that domain knowledge, when embedded into the surrogate modeling strategy-via kernel choice, fidelity layering, or constraint encoding-greatly enhances the optimization outcome and generalization performance.

V. DISCUSSION AND PRACTITIONERS GUIDE

To effectively apply Gaussian Process-augmented Particle Swarm Optimization (GP-PSO), practitioners should adopt key strategies related to model fidelity, parameter tuning, and reproducibility. When possible, multi-fidelity surrogate models should be employed to integrate low-cost approximations with limited high-fidelity evaluations, significantly improving efficiency [55]. In single-fidelity setups, careful kernel selection is essential-e.g., Matérn or ARD kernels-for capturing the underlying function characteristics. Regular re-training of the surrogate, guided by cross-validation or log marginal likelihood, helps maintain prediction quality throughout the optimization process.

In configuring the PSO component, adaptive parameter control is recommended. Dynamic inertia weights and cognitive/social coefficients can enhance swarm behavior by balancing exploration and exploitation. For acquisition functions, Expected Improvement (EI) suits well-rounded objectives, UCB promotes exploratory sampling, and PI offers stable performance in noise-sensitive tasks.

Reproducibility requires explicit documentation of all algorithmic settings-random seeds, PSO parameters, GP training routines, and surrogate configurations. Performance

should be reported using statistical metrics (e.g., mean and standard deviation over multiple runs), and open benchmarks such as CEC or BBOB should be used for comparison. As emphasized by Bi et al. (2022), transparency in experimental protocols and public sharing of code are vital for credible and reproducible optimization research [55].

Table 2. Performance of GP-PSO in real-world engineering applications

Domain	GP-PSO Role	Evaluation Reduction	Convergence Improvement	Key Insight
FOPID robot control	Simulation-guided optimization	~60%	>40%	Enabled low-sample robust controller design [53]
Composite structures	Multi-scale dynamic optimization	45%	30%	Used GP-Pareto front prediction for layered composites [54]
Production scheduling	Parameter optimization under constraints	50–55%	35%	Applied GP to identify priority zones in early iterations [49]
Rock mass modeling	Surrogate for simulation-driven PSO	~40%	~25%	Used dynamic GP updates to reduce sampling [50]

VI. FUTURE DIRECTIONS

Three key challenges will shape the evolution of Gaussian Process-augmented PSO (GP-PSO). First, there is a growing demand for online surrogate learning, where the GP model is updated continuously rather than in fixed batches. This is crucial for dynamic environments such as robotics and real-time control systems. Zhu et al. (2023) highlight the need for responsive surrogates that adapt as data streams in [56].

Second, the lack of formal convergence theory for GP-PSO remains a significant gap. Most theoretical results assume access to exact objective functions, which is not the case in surrogate-guided optimization. Zhang et al. (2020) note that surrogate-induced noise complicates the convergence dynamics, and new models are needed to predict behavior under uncertainty [50].

Third, benchmark standardization is essential for fair evaluation and reproducibility. As Bi et al. (2022) stress, consistent benchmarks-ideally adapted from BBOB or CEC suites-should measure not only accuracy but also surrogate error, uncertainty bounds, and evaluation efficiency [55].

VII. CONCLUSION

This review has demonstrated how integrating Gaussian-process surrogates into Particle Swarm Optimization (GP-PSO) dramatically reduces expensive fitness evaluations-by 30–70 % in benchmarks-while maintaining or improving solution quality. Our three-axis taxonomy (integration strategy, infill criterion, fidelity paradigm) provides a unified framework for understanding methods ranging from deep-kernel GPs and sparse approximations to adaptive retraining and hybrid transfer-learning extensions. From synthetic tests to real-world cases in aerodynamics, structural health monitoring, and chemical-process tuning, GP-PSO consistently delivers 20–50 % faster convergence, guiding

practitioners to select kernels, acquisition functions, and fidelity schemes suited to their problem's cost and dimensionality. Looking forward, enabling online surrogate updates for dynamic environments, establishing rigorous convergence theory under surrogate uncertainty, and standardizing benchmark platforms will be crucial for advancing robust, self-tuning GP-PSO variants in next-generation engineering optimization.

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