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**GOPS: efficient RBF surrogate global optimization algorithm with high dimensions and many parallel processors including application to multimodal water quality PDE model calibration.** (English) Zbl 1478.90098


Summary: This paper describes a new parallel global surrogate-based algorithm Global Optimization in Parallel with Surrogate (GOPS) for the minimization of continuous black-box objective functions that might have multiple local minima, are expensive to compute, and have no derivative information available. The task of picking \( P \) new evaluation points for \( P \) processors in each iteration is addressed by sampling around multiple center points at which the objective function has been previously evaluated. The GOPS algorithm improves on earlier algorithms by (a) new center points are selected based on bivariate non-dominated sorting of previously evaluated points with additional constraints to ensure the objective value is below a target percentile and (b) as iterations increase, the number of centers decreases, and the number of evaluation points per center increases. These strategies and the hyperparameters controlling them significantly improve GOPS’s parallel performance on high dimensional problems in comparison to other global optimization algorithms, especially with a larger number of processors. GOPS is tested with up to 128 processors in parallel on 14 synthetic black-box optimization benchmarking test problems (in 10, 21, and 40 dimensions) and one 21-dimensional parameter estimation problem for an expensive real-world nonlinear lake water quality model with partial differential equations that takes 22 min for each objective function evaluation. GOPS numerically significantly outperforms (especially on high dimensional problems and with larger numbers of processors) the earlier algorithms SOP and PSD-MADS-VNS (and these two algorithms have outperformed other algorithms in prior publications).

**MSC:**

90C26 Nonconvex programming, global optimization
90C30 Nonlinear programming
90C59 Approximation methods and heuristics in mathematical programming
90C66 Derivative-free methods and methods using generalized derivatives
65K05 Numerical mathematical programming methods

**Keywords:**

PDE-constrained optimization; surrogate models; parallel computing; water quality models; global optimization; multi-modal and black-box objective

**Software:**

MISO; MultiMin; MPI; NOMAD; GOPS; Delft3D-WAQ; MIKE SHE; ELCOM; MLMSRBF; EGO; pySOT

**Full Text:** DOI

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