BOF Days

February 10 - 12, 2026

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  - Enhance user experience and integration within the broader ecosystem
- **Outward-facing activities:** Community engagement and discovery
  - Curate and evolve the software portfolio
  - Help teams connect with and grow their user communities
  - Enable the broader community to discover and adopt useful software

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Autotuning HPC Codes and ML Pipelines with GPTune

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Feb 11, 2026
CASS BOF DAYS

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Autotuning

- Problem

Given a target problem (task) and a parameterized code to solve it, find the parameter configuration (combination of parameter values) that optimizes the code performance

  - Metrics: solution time, memory or energy usage, etc. (or combined)

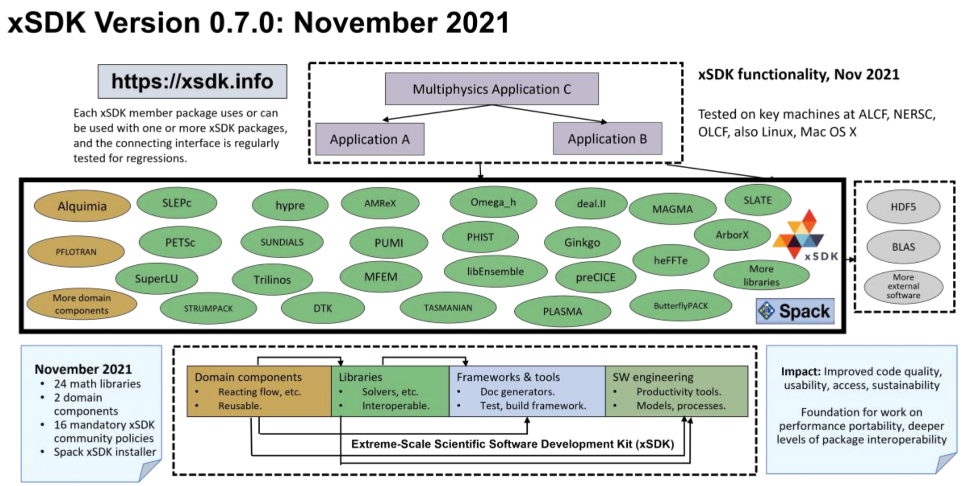
- Real application codes are costly
  - Run on large supercomputers, for a long time

- Real datasets can be large
  - Streaming measurement data can be large
  - Online shared database

- Goal: make best use of limited budget and available data

Applications of GPTune

- Tuning mathematical software on exascale computing platforms



xSDK: Extreme-scale Scientific Software Development Kit (figure obtained from https://xsdk.info/packages/)

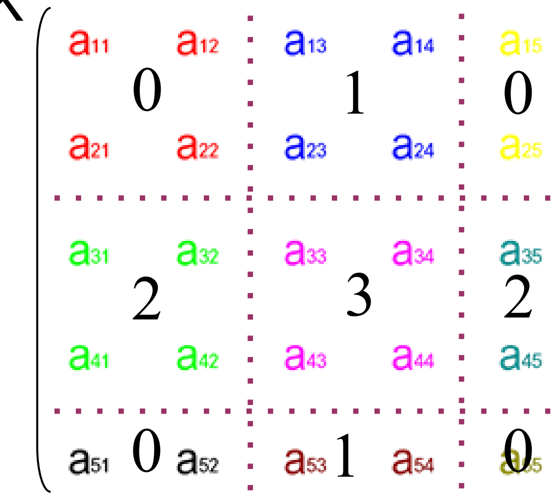
- Tuning computational science codes and experimental control
  - Fusion simulation: NIMROD, M3DC1
  - Electromagnetics simulation: cavity modeling, photonics crystal simulation
  - Accelerator physics: RHIC beamline

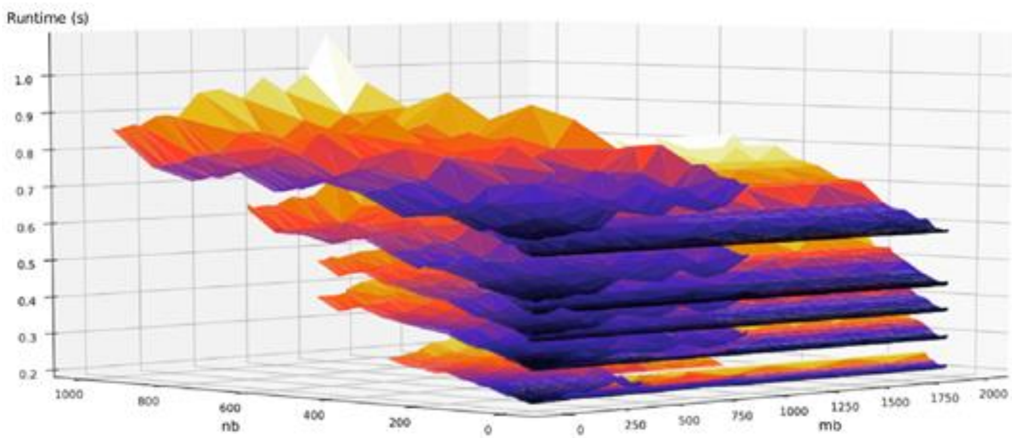
- Physics-informed uncertainty quantification
  - Poisson equation, wave equations, etc.

Example: semi-exhaustive search

$m = n = 5, mb = nb = 2, p$=2

- Parallel dense QR factorization in ScaLAPACK
- 2D block-cyclic layout
- Task is defined by [m, n] pair
- 3 Parameters: {mb, nb, p} (nprocs = pxq)





1 node, 24 cores
$m = n = 2000$
x-axis: mb, y-axis: nb
each layer is one *pxq* config.

- Rule of thumb for best performance (from algorithm viewpoint)
  - Process grid as square as possible
  - Blocks as square as possible

https://github.com/gptune/GPTune

Example: semi-exhaustive search

$m = n = 5, mb = nb = 2, p=2$

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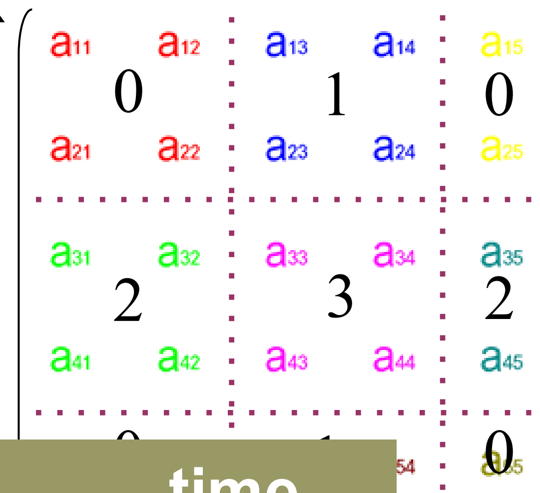

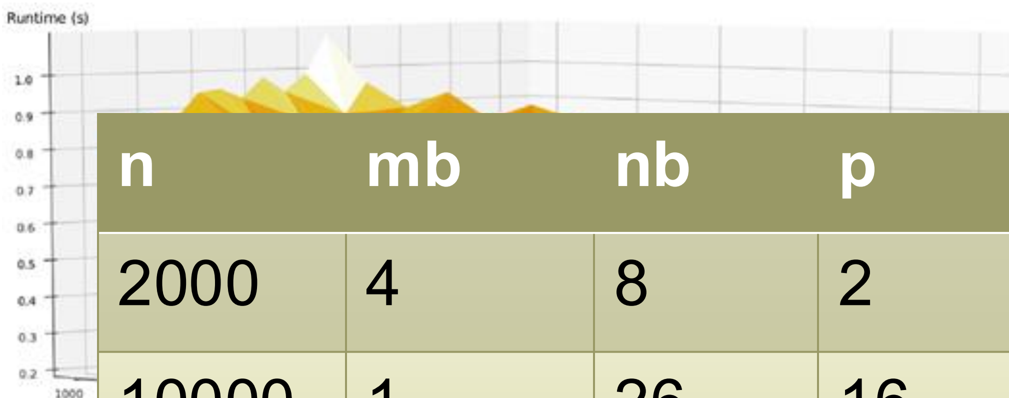

n	mb	nb	p	q	time
2000	4	8	2	12	0.20
10000	1	26	16	192	1.61

- Rule of thumb for best performance (from algorithm viewpoint)
  - Process grid as square as possible
  - Blocks as square as possible

Characteristics of the optimization problems

- No analytical formulation of
  - objective function (runtime, memory, energy, …)
  - gradient
  - problem constraints

- Function evaluation == expensive application run (up to weeks!)
  - large variability related to hardware (e.g., network, disk I/O)

- Non-convex problems and non-linear constraints

- Discrete and continuous search spaces
  - Parameters can be *Real, Integer, Categorical*

Bayesian optimization

- Problem: $\min_x y(x)$, x : parameter configuration
- Bayesian statistical inference is an iterative model-based approach
  - versatile framework for black-box derivative-free global optimization

Sampling: $y_1 \ldots y_{n_0}$

Prior distribution

Surrogate Model $f(x)$

$\min f \approx \min y$

Update Posterior Distribution

Search Next:

$x_{n+1} \rightarrow y_{n+1}$

To optimize Acquisition Function

$p(y) = \mathcal{N}(\mu_0, \Sigma_0)$

Multivariate normal dist.

Bayes Rule

Update model with new data

Bayesian optimization

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To optimize Acquisition Function

Update model with new data

$p(y) = \mathcal{N}(\mu_0, \Sigma_0)$

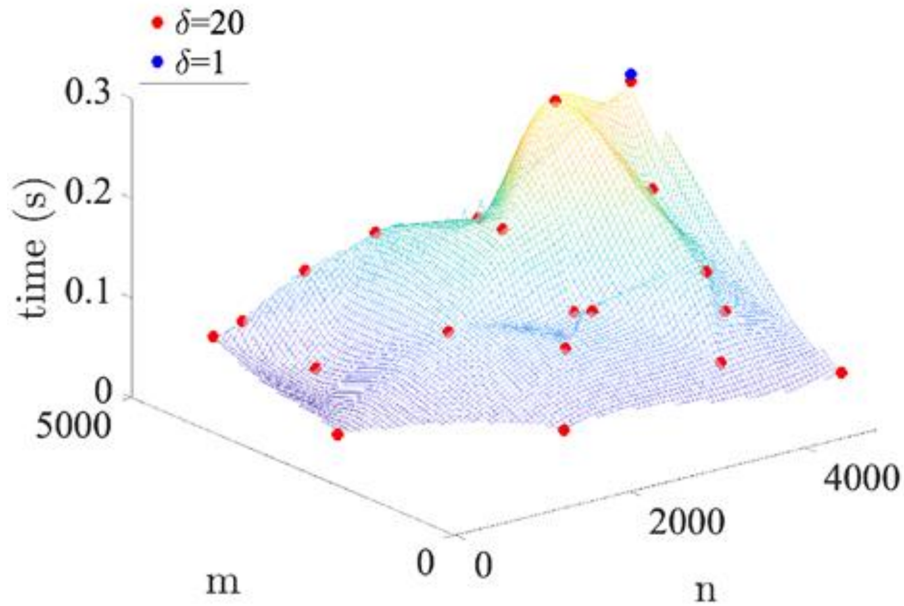
Multivariate normal dist.

Bayes Rule

- Sampler: Monte Carlo Sampling, Latin hypercube sampling, etc.

- Models: Kernels (RBF, Exponential, Matern, Wendland), LCM, multi-armed bandit, clustering, MCTS, transfer learning, etc.
- Optimization: LBFGS, MCMC

- Acquisition Function: Expected Improvement (EI), UCB, MSPE, etc.
- Optimization: GA, PSO, CMA-ES, LBFGS, etc.



Modeling

Gaussian Process Regression

"Gaussian Processes for Machine Learning", Rasmussen and Williams 2006

Modeling: Gaussian Process with e.g. RBF Kernels

- GP defines a distribution over functions, and inference takes place in the space of functions
  - Every finite subset of variables follows multivariate normal distribution
- GP is specified by the mean function and covariance function $k(x, x')$ (kernel)

$$f(x) \sim GP\big(\mu(x), k(x, x')\big)$$
$$\mu(x) = \mathbb{E}[f(x]$$
$$k(x, x') = \mathbb{E}[(f(x) - \mu(x))(f(x') - \mu(x'))]$$

- RBF kernel

$$k(x, x') = \ \sigma^2 \exp(-\sum_{i=1}^{D} \frac{(x_i - x_i')^2}{l_i})$$

covariance is large if two points are close

$$-l(\theta) = \frac{1}{2}\log|K| + \frac{1}{2}(y-\mu)^T K^{-1}(y-\mu) + \frac{n}{\pi}\log(2\pi) \qquad -\nabla l(\theta)_j = \frac{1}{2}\mathrm{tr}\big(K^{-1}\partial_j K\big) - \frac{1}{2}y^T K^{-1}\partial_j K K^{-1} y$$

Hyperparameter $\theta = (\sigma^2, l_i,$ etc.) optimization: MLE, MCMC, etc.

Modeling: GP model prediction

- Given s observation pairs:

$$X = [x^1, x^2, \dots, x^s] \quad Y = [y(x^1), y(x^2), \dots, y(x^s)]$$

Add new point x^*, posterior prob. distribution is : $p(y^*|X) = \mathcal{N}(\mu_*, \sigma_*^2)$
mean (prediction) and variance (confidence) for $y(x^*)$ are:

$$\mu_* = K(x^*, X)\, K(X, X)^{-1}\, Y$$
$$\sigma_*^2 = K(x^*, x^*) - K(x^*, X)\, K(X, X)^{-1} K(x^*, X)^T$$

Dimension of covariance matrix $K(X, X)$ = number of samples

Inversion of K and its log determinant can be quite expensive to compute

Modeling: Other Kernels, Optimizers and Algorithms

Tuner	Kernel, modeler	Model optimizer	Fast inversion	Acquisition function	Search algorithm
GPTune (single-objective)	RBF, Exponential, Matern, LCM, WGP	lbfgs	ScaLAPACK	EI, UCB, MSPE, q-UCB, q-EI	pso, ga, cmaes, l-bfgs-b, dual_annealing, trust-constr,shgo
GPTune (multi-objective)	RBF, Exponential, Matern, LCM	lbfgs	ScaLAPACK	EI, UCB, MSPE, q-UCB, q-EI, UCB-HVI†	nsga2, nspso, maco, moead
GPTuneBand	LCM and multi-armed bandit	lbfgs	ScaLAPACK	EI, UCB	pso, successive halving
cGP	Matern and clustering	lbfgs, MCMC	N/A	EI, MSPE	lbfgs
GPTuneHybrid	Matern and MCTS	lbfgs	N/A	GP-EI, GP-UCB, UCTS, Multinomial	lbfgs
GPTuneGeorge	RBF, Matern, LCM, sparse kernels	lbfgs, MCMC	HODLR, SuperLU_DIST	EI, UCB, MSPE, q-UCB, q-EI	pso, ga, cmaes, l-bfgs-b, dual_annealing, trust-constr,shgo

Table 2: Algorithm components of each supported tuner in GPTune. †: UCB-HVI uses the same search algorithm as in GPTune (single-objective).

Search Phase

- Where to place the new sample point?
  - Maximize certain Acquisition Function
  - Optimization based on surrogate model (easier!)

- Balance between exploitation and exploration
  - **Exploitation**: local search within promising regions
  - **Exploration**: global search of new regions with more uncertainty

- Given a new sample point, need quickly update the model

Acquisition Function (1)

- **Expected Improvement (EI)** – most commonly used AF

For a new point x^*, expected difference from current best is

$$I(x) = \max(y^{min} - f(x^*),\ 0)$$

$$EI(x^*) = \mathbb{E}\big(I(x)\big) = (y^{min} - \mu(x^*))\ \Phi(Z) + \sigma(x^*)\phi(Z)$$

- $Z = \frac{y^{min} - \mu(x^*)}{\sigma(x^*)}$
- $\Phi(.)$ = CDF of the standard normal distribution
- $\phi(.)$ = PDF of standard normal distribution

[Jones et al. 1998]

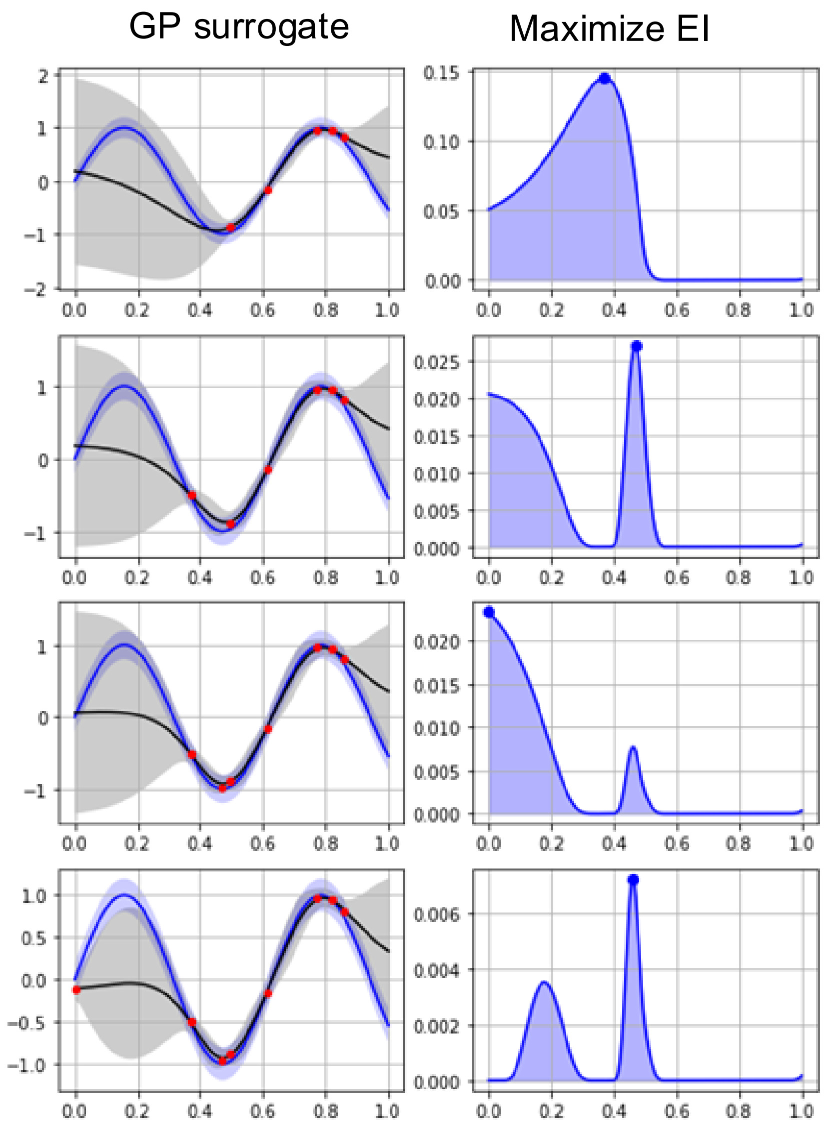
Acquisition Function (2)

- **Lower Confidence Bound (LCB)**

$$x^* = argmin_x \, LCB(x) = \mu(x) - \lambda \, \sigma(x)$$

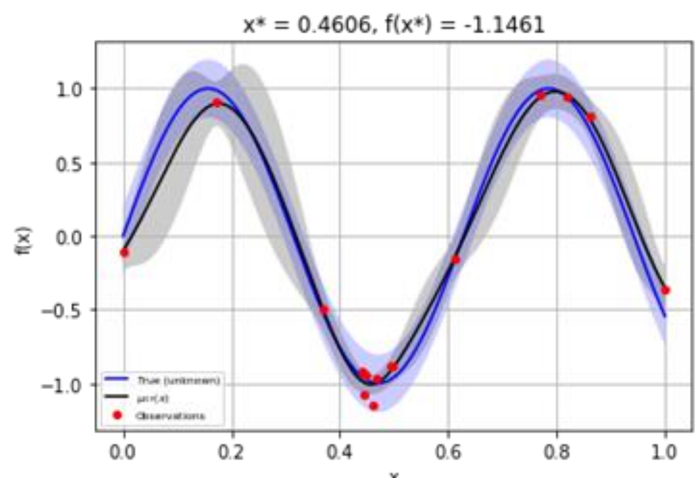
- $\mu(x) \rightarrow$ exploitation: favor points predicted to have low values
- $-\lambda\sigma(x) \rightarrow$ exploration: subtracting uncertainty, prefer points where the lower bound could be much smaller than the mean
- $\lambda \rightarrow$ trade-off parameter controlling exploration vs exploitation

1D example: black-box function $y(x) = sin(10x)$



5 initial samples
4 additional steps

- Blue line: true function
- Red dots: function evaluations
- Black line: mean function of the fitted surrogate model
- Grey shaded area is 95% confidence interval



Search: Other Acquisition Functions and Algorithms

Tuner	Kernel, modeler	Model optimizer	Fast inversion	Acquisition function	Search algorithm
GPTune (single-objective)	RBF, Exponential, Matern, LCM, WGP	lbfgs	ScaLAPACK	EI, UCB, MSPE, q-UCB, q-EI	pso, ga, cmaes, l-bfgs-b, dual_annealing, trust-constr,shgo
GPTune (multi-objective)	RBF, Exponential, Matern, LCM	lbfgs	ScaLAPACK	EI, UCB, MSPE, q-UCB, q-EI, UCB-HVI†	nsga2, nspso, maco, moead
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Table 2: Algorithm components of each supported tuner in GPTune. †: UCB-HVI uses the same search algorithm as in GPTune (single-objective).

GPTune Software: github.com/gptune/GPTune

- Python interface, leverage existing Python packages
  - GPy, scipy, scikit-learn, scipy, scikit-optimize, MPI4py, pymoo, pygmo …
- HPC code for parallel covariance matrix computation/inversion: BLAS, ScaLAPACK, ButterflyPACK, George, SuperLU_DIST
- Part of xSDK, E4S, spack

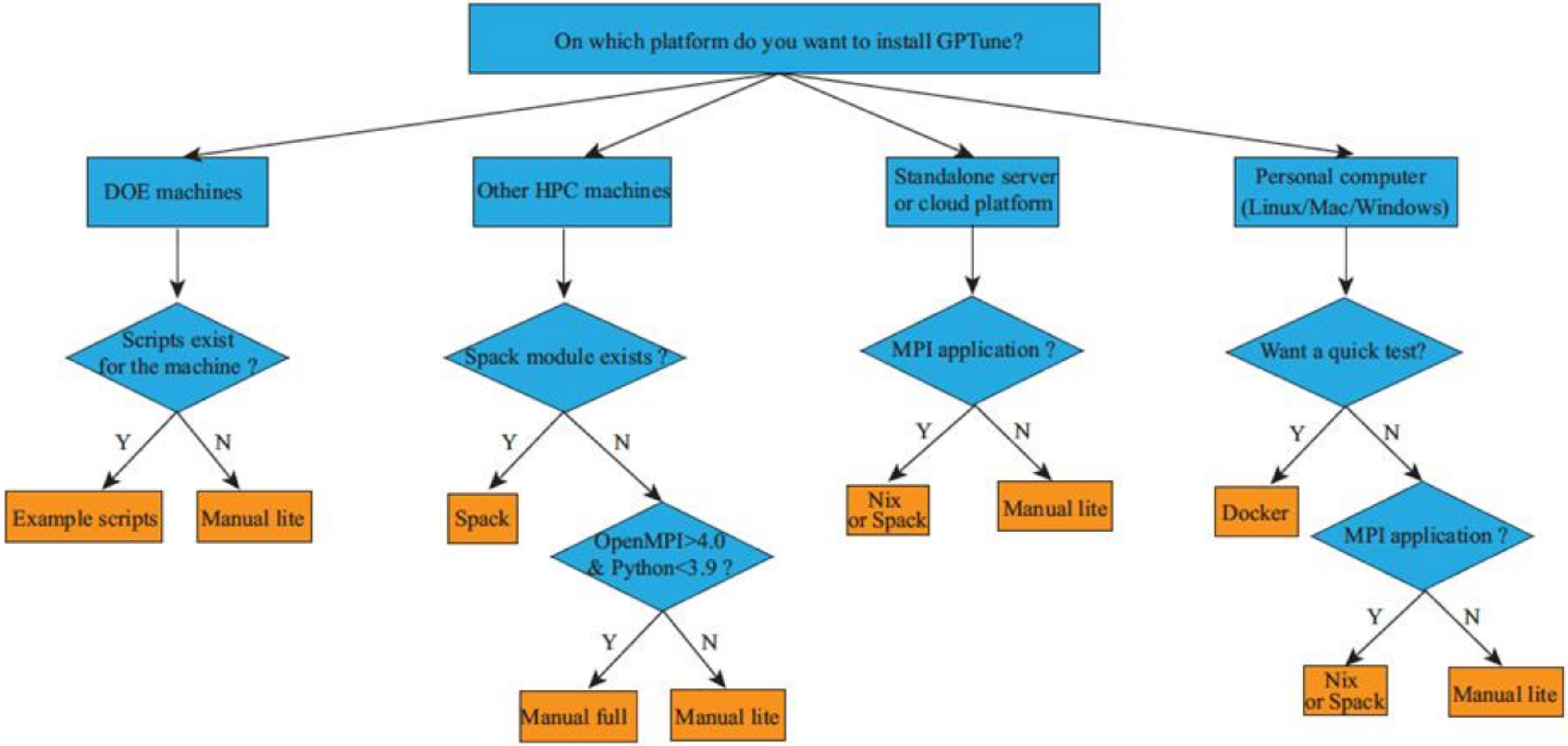
- User input:
  - Task parameter input space ( ): the space of tasks parameters
    - QR example: m = n = 20000
  - Tuning parameter space ( ): the space of tuning parameters
    - (categorical, integer, real), and ranges
    - QR example: {mb, nb, nprow}
  - Output space ( ): the space of objective function values
    - runtime
  - Define application as a black-box function
    - Python to C / Fortran interface

(Optionally)

- Define constraints in parameter search space
- Define performance models
- Choose a search method
- ……

GPTune Software: Installation Options

- Manual full, manual lite, Spack, Nix, Docker
- For quick test, use the Docker image https://ggle.io/5X02



https://github.com/gptune/GPTune

Easy-to-Use Interface in Python

A model problem to illustrate user interface

$$y(t,x) = sin(10x + 2t)$$

3 tasks: $t = 0, 0.5, 1.0$

Use Python classes to:

- Express arbitrary complex sets of constraints
- Provide arbitrary sets of tuning choices, as first class objects

```
from autotune.problem import *
from autotune.space import *
from autotune.search import *
from GPTune.gptune import *
```

Import internal Python classes

```
….
input_space = Space( [Real(0., 10., name="t")] )
parameter_space = Space( [Real(0., 1., name="x")] )
output_space = Space( [Real(-Inf, Inf, name="y")] )
```

Define application parameters (categorical, integer, real) and ranges

```
def objectives(point):
    t = point['t']
    x = point['x'];
    f = np.sin(10*x + 2*t)
    return [f]
```

Define application as a black-box function

```
constraints = {"cst1": "x >= 0. and x <= 1."}
```

***Define constraints in parameter search space** [optional]*

```
def analytical_model1(point):
    f = np.sin(10*x + 2*t)
    return [f*(1+np.random.uniform()*0.1]
models = {'model1': analytical_model1}
```

***Define performance models** [optional]*

```
constants={"AAA":aaa,"BBB":bbb}
```

***Define constants** [optional]*

```
problem = TuningProblem(input_space, parameter_space,
output_space, objectives , constraints, models, constants)
```

```
options = Options()
options['XXX'] = 'YYY'
```

Set GPTune options

```
gt = GPTune(problem, computer, data, options, … )
gt.MLA(NS, giventask, NI, NS1=int(NS/2))
```

Use different tuners

https://github.com/gptune/GPTune

Unified interface to many tuners

- External tuners: opentuner, hpbandster, etc.
- Our tuners: GPTune, GPTuneBand, cGP, GPTuneHybrid, etc.

```
# Define objectives, constraints, spaces, options, computer
...
# Define the "autotune" interface to all tuners
problem = TuningProblem(IS, PS, OS, objectives, constraints)
# Call different tuners
if(TUNER_NAME=='GPTune'):
    gt = GPTune(problem, computer=computer, options=options)
    (data, model, stats) = gt.MLA(NS=NS, Igiven=giventask)
if(TUNER_NAME=='opentuner'):
    (data,stats)=OpenTuner(T=giventask,NS=NS,problem,computer)
if(TUNER_NAME=='hpbandster'):
    (data,stats)=HpBandSter(T=giventask,NS=NS,problem,computer)
if(TUNER_NAME=='GPTuneBand'):
    gt = GPTune_MB(problem, computer=computer,NS=1,options=options)
    (data, stats, data_hist)=gt.MB_LCM(NS=1,Igiven=giventask)
if(TUNER_NAME=='cgp'):
    (data,stats)=cGP(T=giventask,problem,computer,options=options)
```

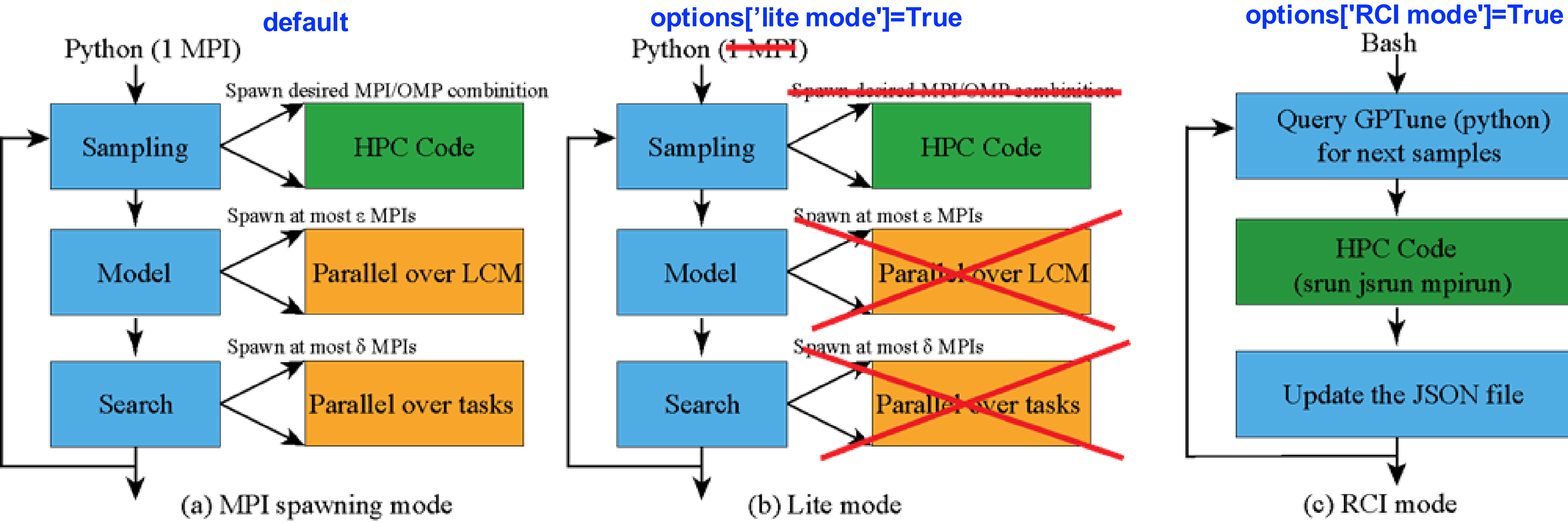
Variants of Algorithms and Features in GPTune

- Multi-task learning algorithm (GPTune MLA): $y(t,x)$, t denotes task parameters
- Transfer learning algorithm (GPTune TLA): from trained $y(t_1,x)$ to improve $y(t_2,x)$
- Multi-fidelity tuning (GPTuneBand): $y(s,t,x)$, s denotes a fidelity level
- Multi-objective tuning (GPTune): $y^l(t,x)$ denotes the l^{th} objective function
- Mixed-variable tuning (GPTuneHybrid)
- Non-smooth objectives (cGP)
- Database, visualization, and crowd tuning (https://gptune.lbl.gov/repo/dashboard/)
- Other features: parallel implementation, checkpointing, sensitivity analysis, importance analysis, coarse performance models

	Tuner	MLA	TLA	multi-fidelity	multi-objective	parallel tuning	database logging	checkpoint & restart
	GPTune	✓	✓		✓	✓	✓	✓
GPTune variants	GPTuneBand	✓		✓		✓	✓	✓
	cGP						✓	
	GPTuneHybrid						✓	
External	HpBandSter						✓	
	OpenTuner						✓	

Parallel architecture of GPTune

- Three execution modes of GPTune: MPI spawning mode, lite mode and reverse communication interface (RCI) mode

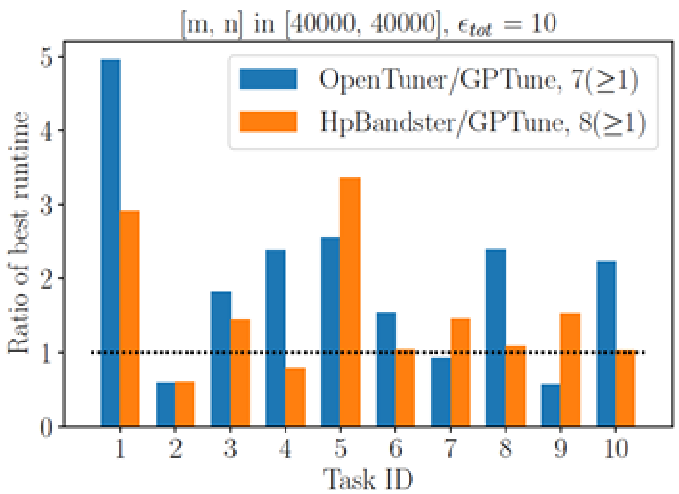


	spawning	lite	RCI
call application	from python	from python	from bash
parallel model/search	yes	no	yes
code instrumentation	yes	no	no

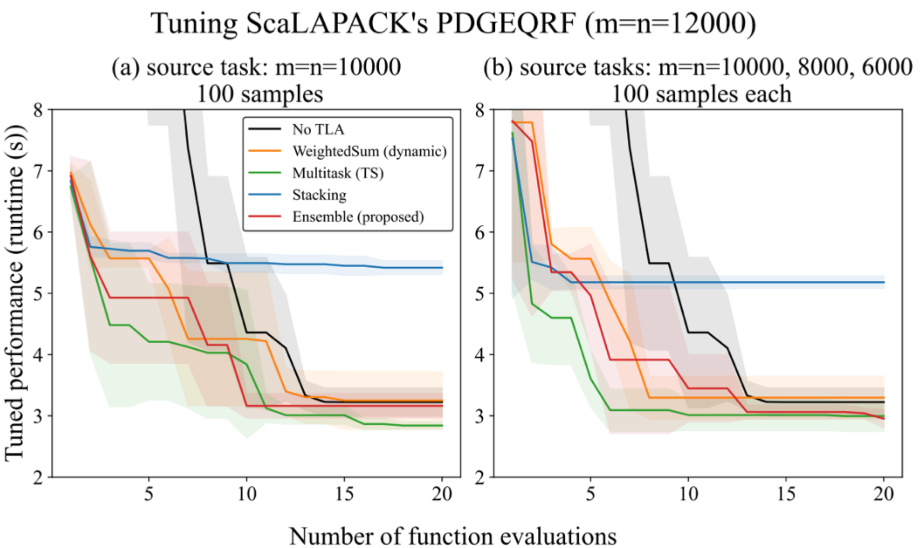
https://github.com/gptune/GPTune

Feature 1: Multitask Learning (MLA) and Transfer Learning (TLA)

- Consider a set of correlated objective functions $\{y_i(X)\}_{i\in 1..\delta}$, we want to tune them all together (MLA) or use the models of $y_i, i = 1,..,\delta-1$ to tune y_δ (TLA).
- Both MLA and TLA increase the effective number of samples



MLA tuning runtime of ScaLAPACK QR of 10 matrices

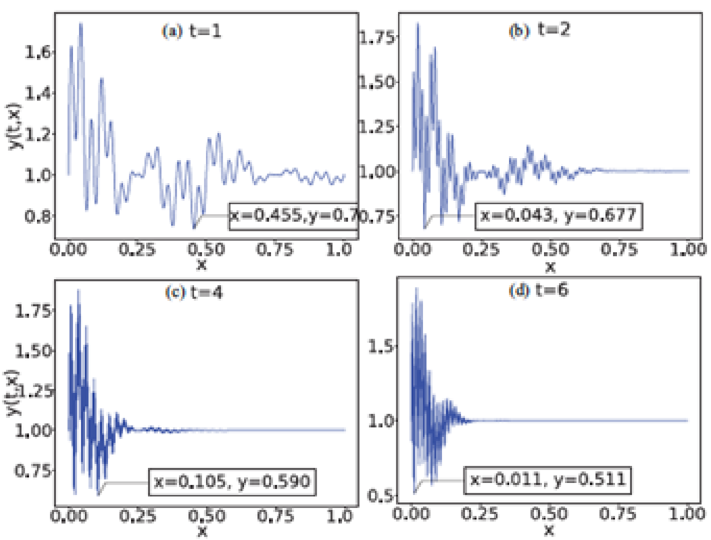


TLA tuning runtime of ScaLAPACK QR of 1 target matrix from 1 source matrix

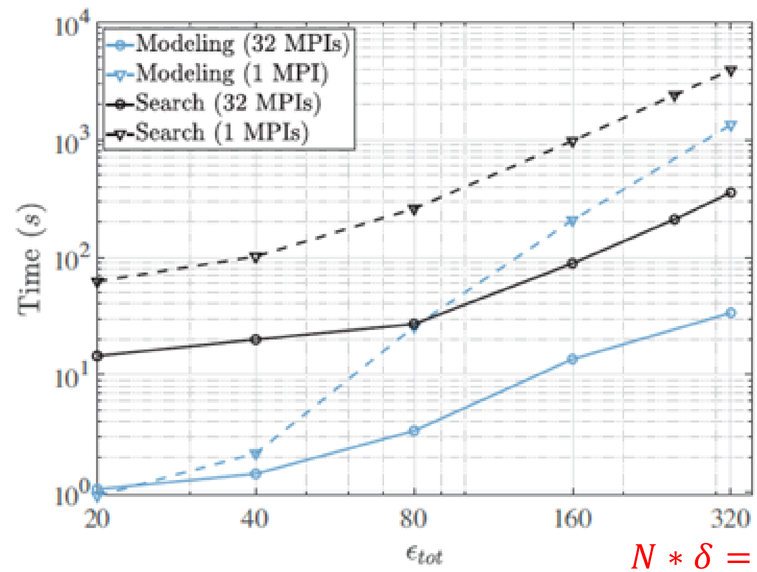
Feature 2: Fast K Computation: ScaLAPACK

Consider an analytical function, t, x: task and tuning parameters, $\delta = 20$ tasks N : number of samples per task.

$$y(t,x) = 1 + e^{-(x+1)^{t+1}} \cos(2\pi x) \sum_{i=1}^{3} \sin\left(2\pi x (t+2)^i\right)$$



Objective functions



$N * \delta = 6400$

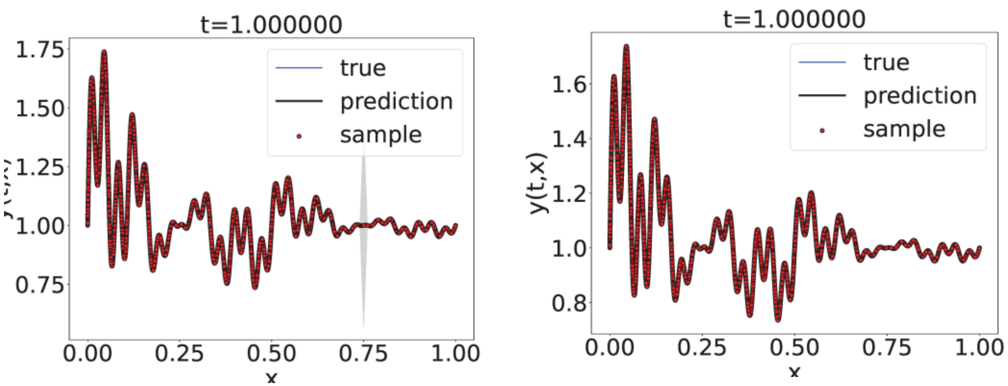
Parallel performance

* GPTune: Multitask learning for autotuning exascale applications, Yang Liu, Wissam M Sid-Lakhdar, Osni Marques, Xinran Zhu, Chang Meng, James W Demmel, Xiaoye S Li, PPoPP'21

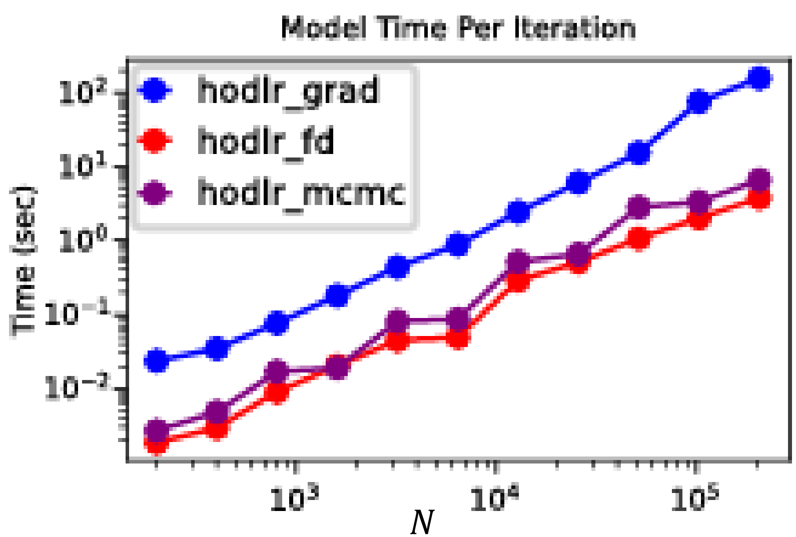
Feature 2: Fast K Computation: Hierarchical Matrices

Idea: leverage low-rank compression to exploit data-sparsity of dense kernel matrices

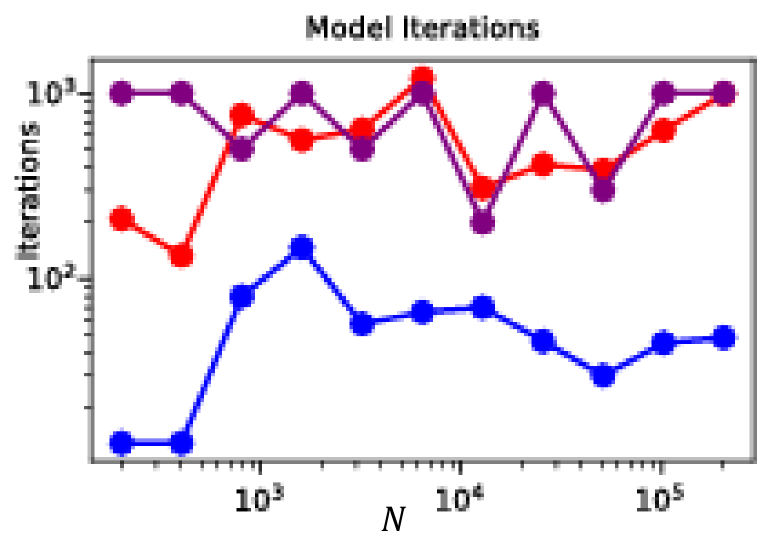
Setup: generate N random samples, build the GP model, and predict the $(N+1)^{th}$ sample



$N = 102400.$
Left: LBFGS.
Right: MCMC



$-l(\theta)$ and $-\nabla l(\theta)_j$ per MCMC or LBFGS iteration



Iteration counts of MCMC or LBFGS

Feature 2: Fast K Computation: Sparse Kernel Computation via SuperLU_DIST

$$k(x,x') = \sigma^2 \exp\left(-\sum_{1=1}^{D}\frac{\left(x_i - x_i^i\right)^2}{l_i^2}\right) \times \left(1-\frac{r}{r_c}\right)^4\left(\frac{4r}{r_c}+1\right)$$

RBF **Wendland**

Negative log-likelihood: (LBFGS, MCMC, etc.)

$$-l(\theta) = \frac{1}{2}\log|K| + \frac{1}{2}(y-\mu)^T K^{-1}(y-\mu) + \frac{n}{\pi}\log(2\pi)$$

The gradient (LBFGS):

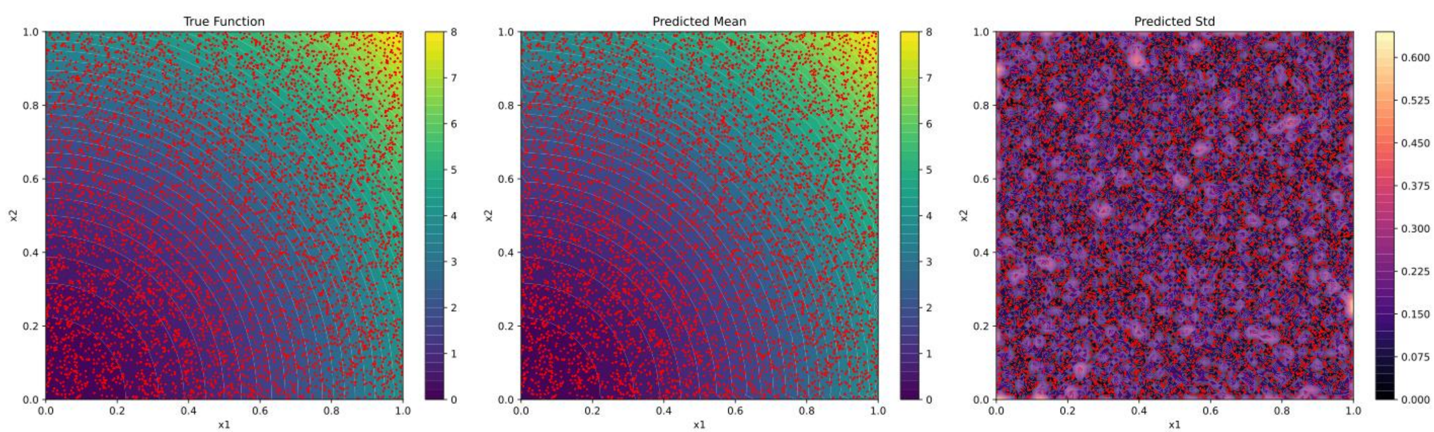
$$-\nabla l(\theta)_j = \frac{1}{2}\mathrm{tr}\left(K^{-1}\partial_j K\right) - \frac{1}{2}y^T K^{-1}\partial_j K K^{-1} y$$

Randomized Hutchinson trace estimator:

$$\mathrm{tr}\left(K^{-1}\partial_j K\right) \approx \frac{1}{m}\sum_{l=1}^{m} u_l^T K^{-1}\partial_j K u_l$$

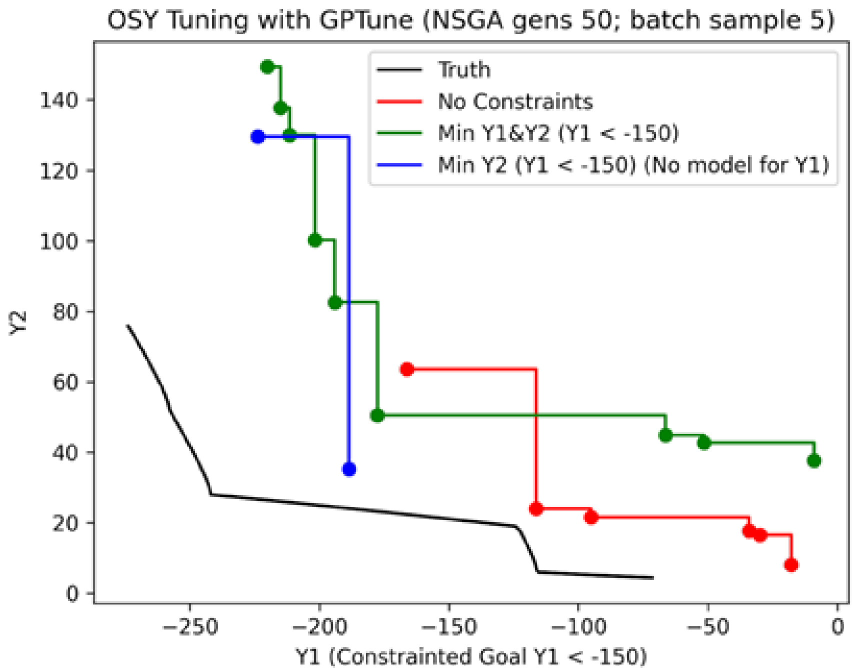
Leverage the newly developed SuperLU_DiST python interface via file-based IO

$N = 6400$



Feature 3: Multi-objective tuning

- Part II.2 of https://ggle.io/5X02
- Pareto optimal: no other PS points dominate over this point in all objectives.
- Unconstrained and constrained multi-objective tuning **output_space = Space([y1, y2, ...])**
  - No constraint, optimize: **yk = Real(float("-Inf"), float("Inf"), name="yk")**
  - Constrained, optimize: **yk = Real(float("-Inf"), 10.0, name="yk")**
  - Constrained, not-to-optimize: **yk = Real(float("-Inf"), 10.0, name="yk", optimize=False)**



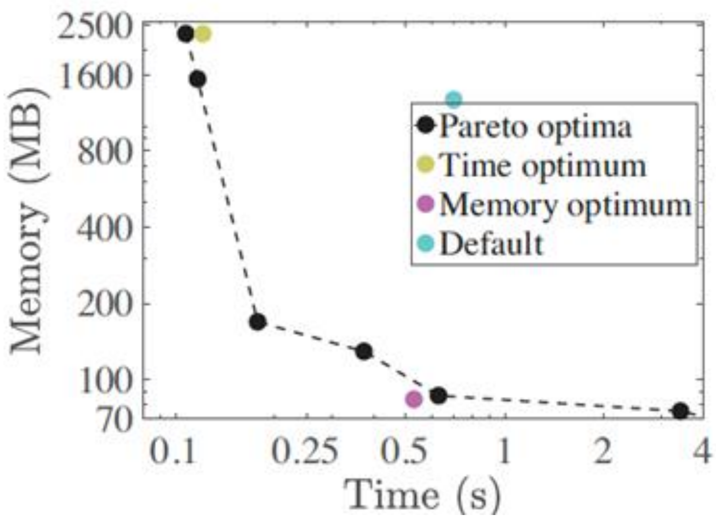
https://github.com/gptune/GPTune

Feature 3: Multi-objective tuning of SuperLU_DIST

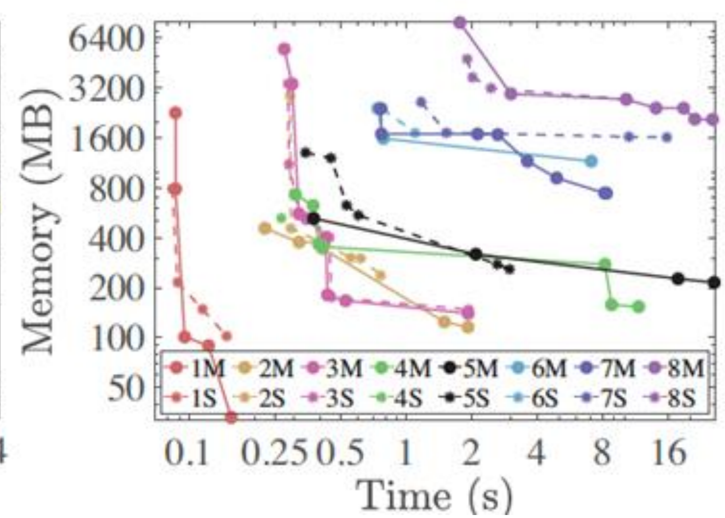
- Unconstrained two objective tuning
- Part II.2 of https://ggle.io/5X02

Multi-objective EGO: One LCM per objective, NSGA-II in search

- $\mathbb{IS}$=[matrix name] $\mathbb{PS}$=[COLPERM, NSUP, NREL, nprows].
- Multi-objective: $\mathbb{OS} = [time, memory]$, single-objective: $\mathbb{OS} = [time]$ or $[memory]$. MLA $\delta = 8$ or single-task. 256 cores.
- Pareto optimal: no other $\mathbb{PS}$ points dominate over this point in both objectives.



single-task



MLA

Feature 4: Incorporation of Coarse Performance Model

- Part II.4 of https://ggle.io/5X02
- An analytical formula can significantly improve tuning performance

A coarse performance model $\tilde{y}(t,x)$ (per task) can be built into $\mathbb{PS}$: $x \rightarrow [x, \tilde{y}(t,x)]$. $\tilde{y}(t,x)$ can also be parameterized.

A simple performance model for PDGEQRF

$$\tilde{y}(t,x) = C_{flop} \times t_{flop} + C_{msg} \times t_{msg} + C_{vol} \times t_{vol} \quad (1)$$

with the number of floating point operations C_{flop}, the number of messages C_{msg} and the volume of messages C_{vol}

$$C_{flop} = \frac{2n^2(3m-n)}{2p} + \frac{b_r n^2}{2p_c} + \frac{3b_r n(2m-n)}{2p_r} + \frac{{b_r}^2 n}{3p_r} \quad (2)$$

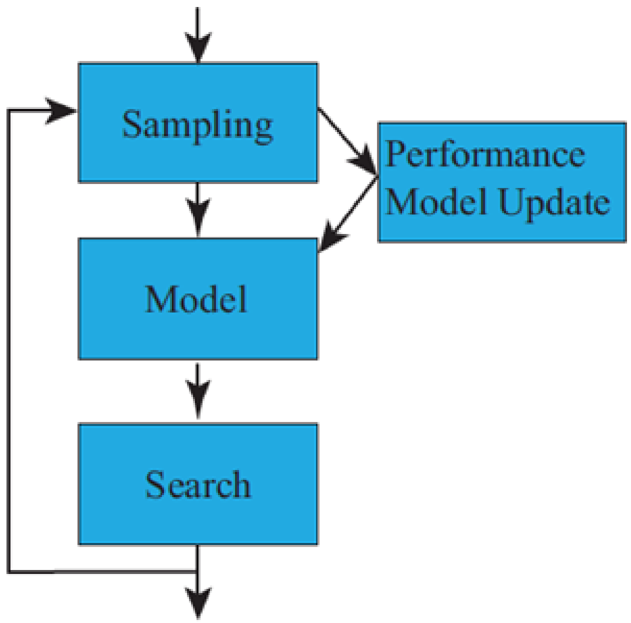
$$C_{msg} = 3n \log p_r + \frac{2n}{b_r} \log p_c \quad (3)$$

$$C_{vol} = \left(\frac{n^2}{p_c} + b_r n\right) \log p_r + \left(\frac{mn - n^2/2}{p_r} + \frac{b_r n}{2}\right) \log p_c \quad (4)$$

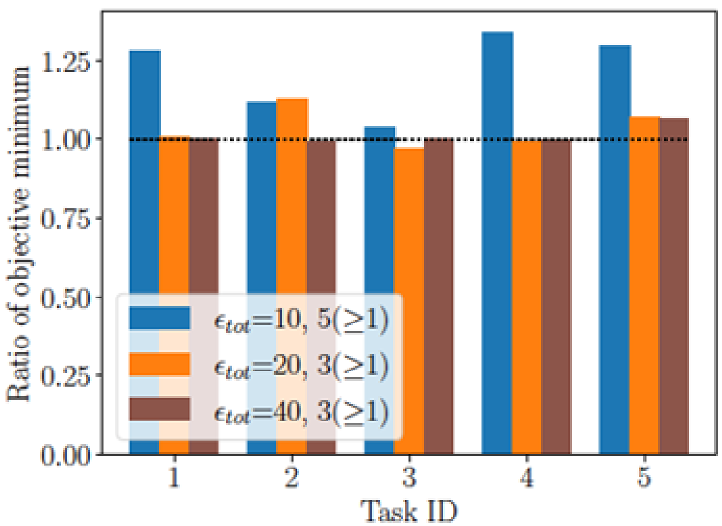
Feature 4: Incorporation of Coarse Performance Model

- An analytical formula can significantly improve tuning performance
- The formula can have hyperparameters as well

A coarse performance model $\tilde{y}(t,x)$ (per task) can be built into $\mathbb{PS}$: $x \rightarrow [x, \tilde{y}(t,x)]$. $\tilde{y}(t,x)$ can also be parameterized.



(a) Incorporate performance model



(b) PDGEQRF: ratio between best runtime with and without the performance model

Feature 5: Multi-fidelity tuning with GPTuneBand

- Part II.5 of https://ggle.io/5X02

Multi-fidelity tuning of hypre

- Convection-diffusion equation on a n^3 grid:
$$-c\Delta u + a\nabla \cdot u = f$$
- $\mathbb{IS}$=[a, c], $\mathbb{PS}$=12 integer/real/categorical, $\mathbb{OS}$=[runtime]
- Fidelity/budget $\sim n^3$.

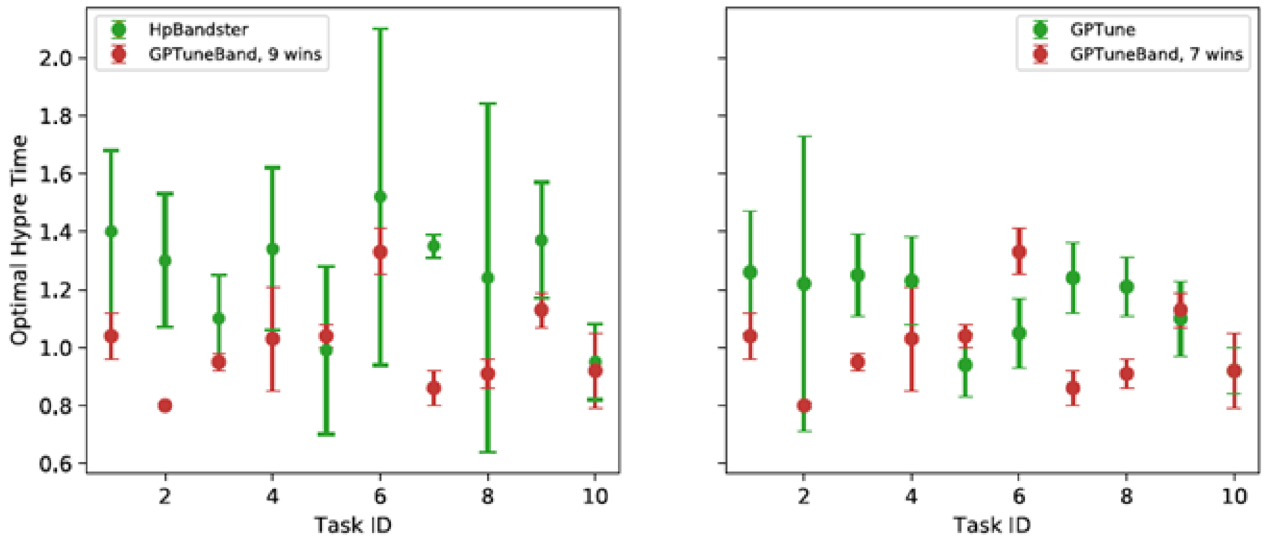
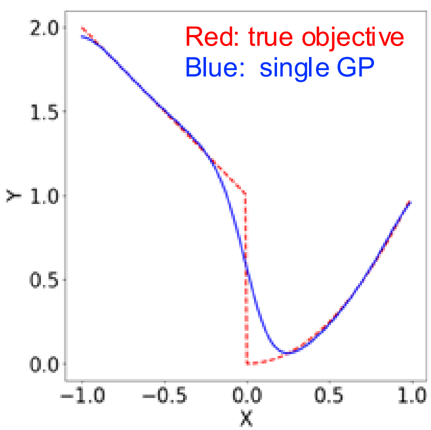
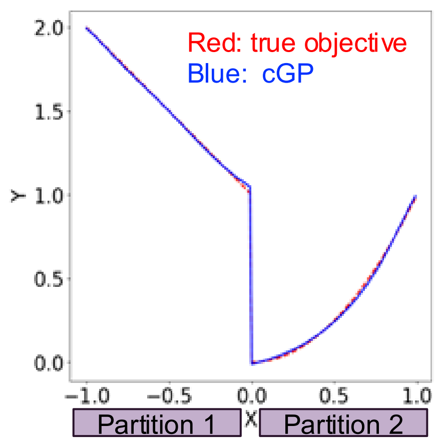


Figure: Comparison of GPTuneBand (multi-fidelity, MLA), GPTune (MLA), and HpBandster (multi-fidelity)

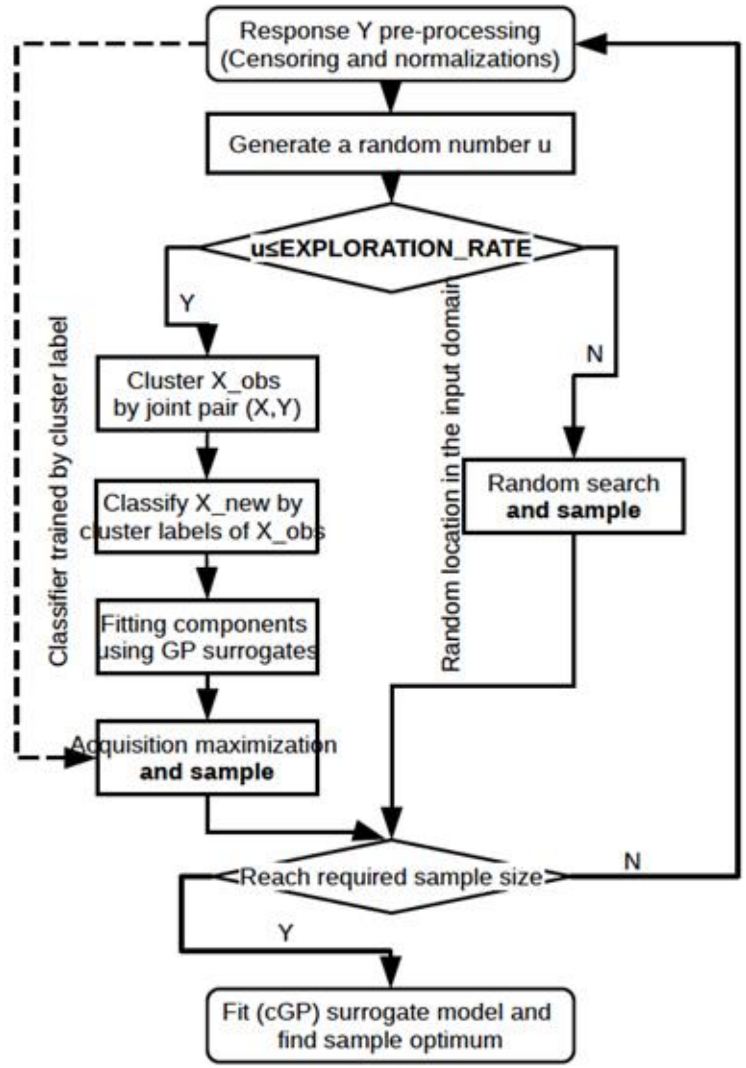
Feature 6: Handling non-smooth objectives with cGP

- Non-smooth objective (discontinuity): single GP performance poor
- cGP (clustered GP): auto-partitioning of the parameter domain and build GP on each





- cGP key options:
  - N_COMPONENT: maximal number of clusters.
  - EXPLORATION_RATE: probability of generating new samples from the acquisition instead of random



cGP workflow

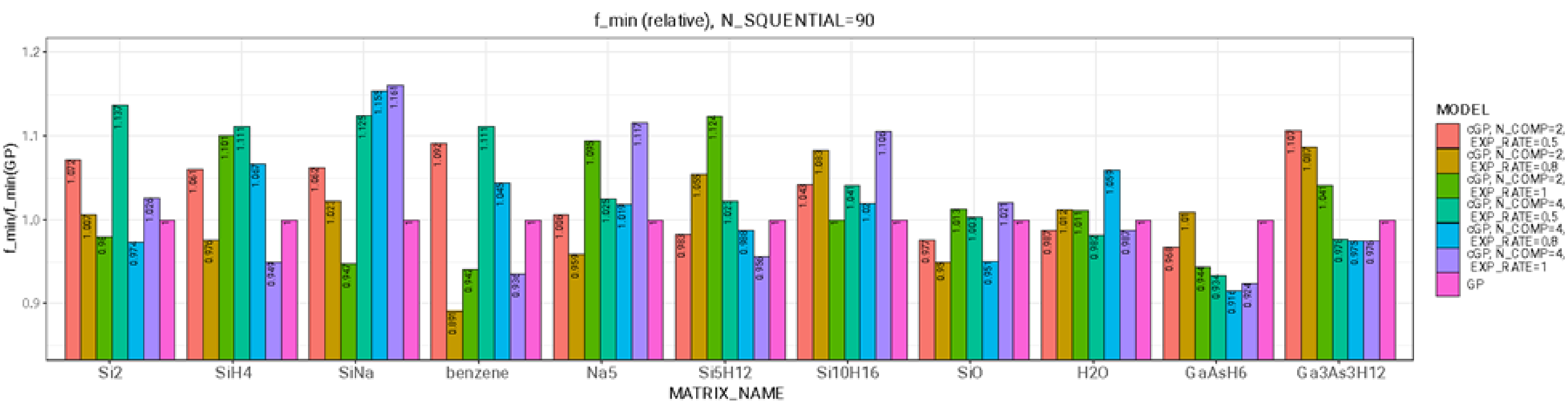
https://github.com/gptune/GPTune

Feature 6: Handling non-smooth objectives with cGP

- Part II.6 of https://ggle.io/5X02

Tuning SuperLU_DIST factorization time

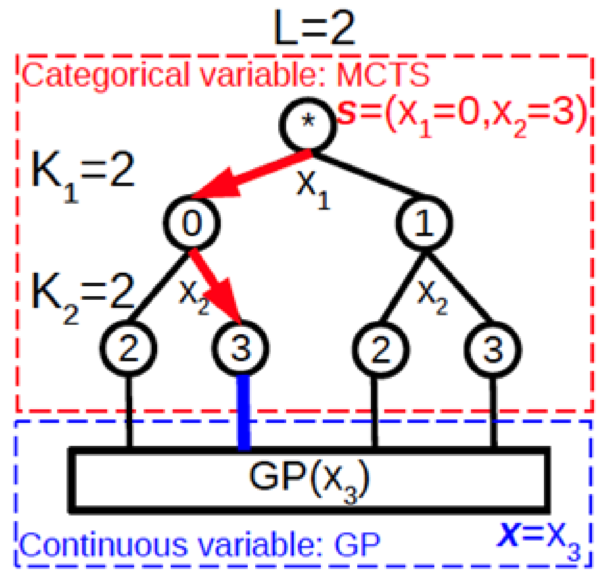
- $\mathbb{IS}$=[matrix name] $\mathbb{PS}$=[NSUP, NREL, nprows].
- Objective: $\mathbb{OS} = [\mathit{time}]$. Single-task. 256 cores.
- N_COMPONENT and EXPLORATION_RATE are performance critical



cGP outperforms single GPs by up to 11.5% for 90% of all 11 matrices

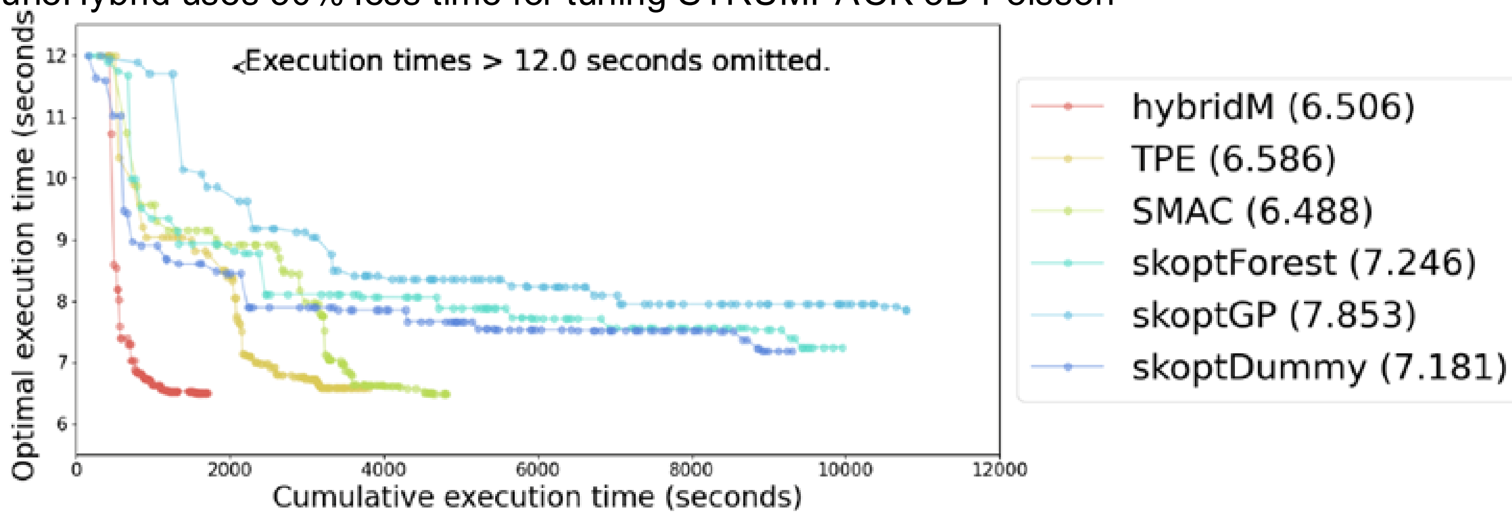
Feature 7: Handling mixed-variables with GPTuneHybrid

- Part II.7 of https://ggle.io/5X02
- Mixed-variable (categorical variables + continuous variables): GP performance poor
- GPTuneHybrid: Monte Carlo Tree Search (MCTS) for categorical variables and GP for continuous variables.



rid workflow

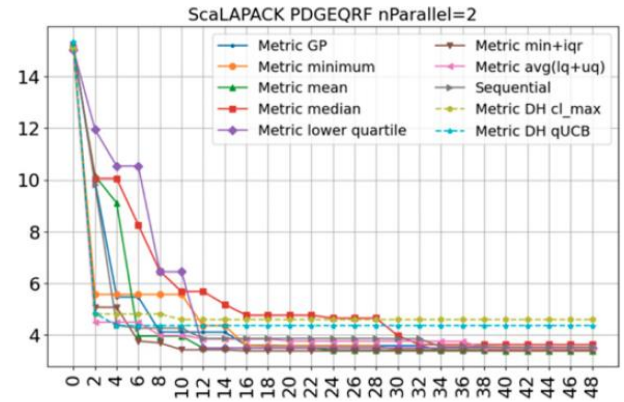
GPTuneHybrid uses 50% less time for tuning STRUMPACK 3D Poisson



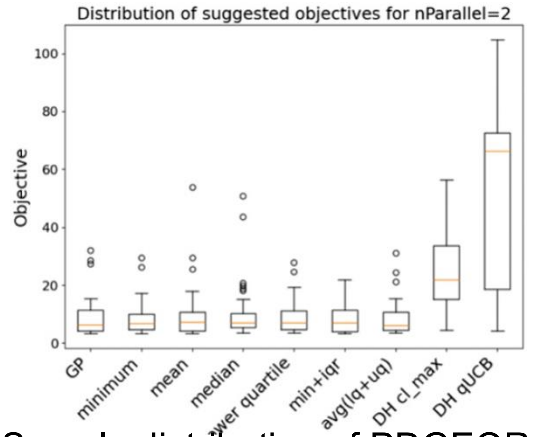
Feature 8: Multiple Sample Generation in the Search Phase

- Goal: generate multiple new samples per BO iteration
  - Reduce the number of hyperparameter optimization model stages (q-EI, not Liar strategy)
  - Leverage distributed-memory parallelism to run multiple function evaluations

- Methods:
  - Multi-point acquisition functions (e.g., q-EI): providing joint expected improvement of q samples.
  - GP-mean-based Liar strategy: use **model predicted mean** as the function value, update the model, after q steps, evaluate the true function.
  - Constant Liar strategies: use **statistical metrics (e.g., min, max, mean, etc.) of existing samples** as the function value, update the model, after q steps, evaluate the true function.



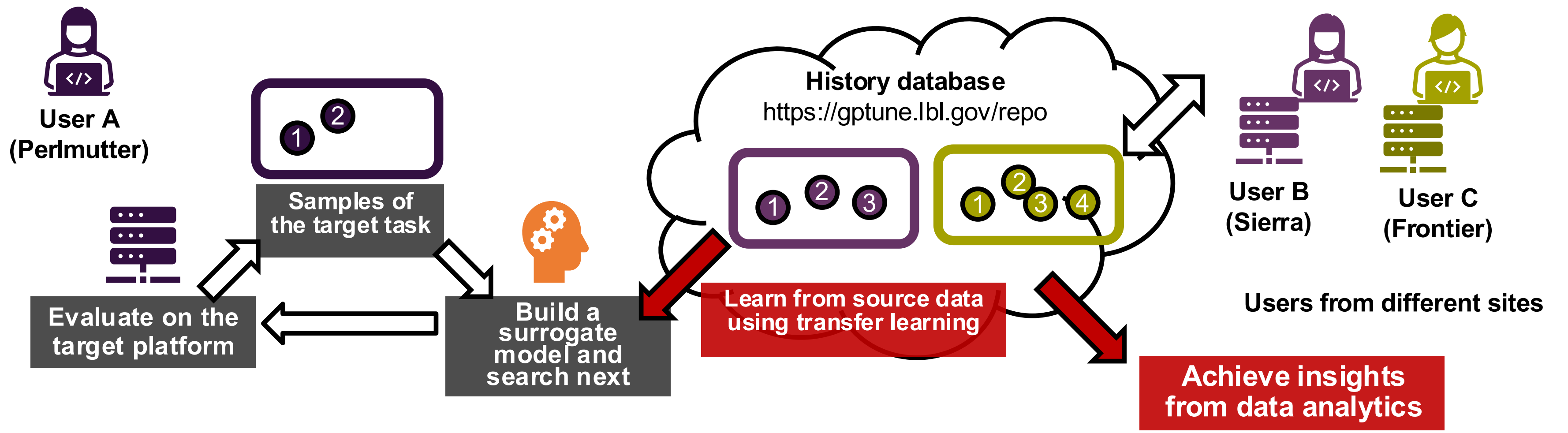
Convergence of PDGEQRF tuning with GPTune and DeepHyper



Sample distribution of PDGEQRF tuning with GPTune and DeepHyper

* Parallelizing autotuning for HPC applications: Unveiling the potential of the speculation strategy in Bayesian optimization, AP Dieguez, S Ockerman, T Aikman, Y Cho, Y Liu, KZ Ibrahim, IJHPCA, 2025

Feature 9: Crowd Tuning: Harnessing the Crowd for Autotuning



- Observation: for popular applications, there are multiple users need tuning
- Our goals:
  1. Build an infrastructure to collect obtained knowledge
  2. Leverage previously collected data for better tuning (fewer evaluations)
  3. Provide useful data analytics from the shared database (history database)

* Harnessing the crowd for autotuning HPC applications, Y. Cho, J. Demmel, J. King, X. S. Li, Y. Liu, H. Luo, IPDPS’23

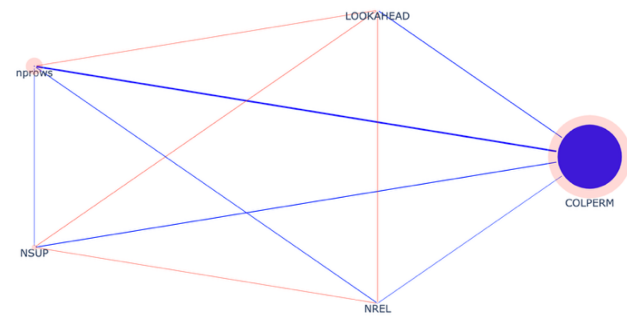
* Enhancing autotuning capability with a history database, Y.Cho, J. Demmel, X. S. Li, Y. Liu, H. Luo, MCSoC’21

Feature 9: Crowd Tuning: Sensitivity Analysis

- Sobol's sensitivity analysis: variance-based analysis to estimate the sensitivity of each variable and interactions of the variables (variable = tuning parameter)
  - **S1: the influence on a single parameter**
  - **ST: the influence of a parameter that includes all interactions with other parameters**
  - **S1/ST_conf: confidence interval**

Matrix: Si5H12	S1	S1_conf	ST	ST_conf
COLPERM	0.795619	0.061109	0.860267	0.070658
LOOKAHEAD	0.004315	0.009732	0.011590	0.002510
nprows	0.109990	0.049130	0.169862	0.032508
NSUP	0.008409	0.021093	0.055794	0.015733
NREL	0.004392	0.008828	0.011989	0.003025

Example result of SuperLU_DIST



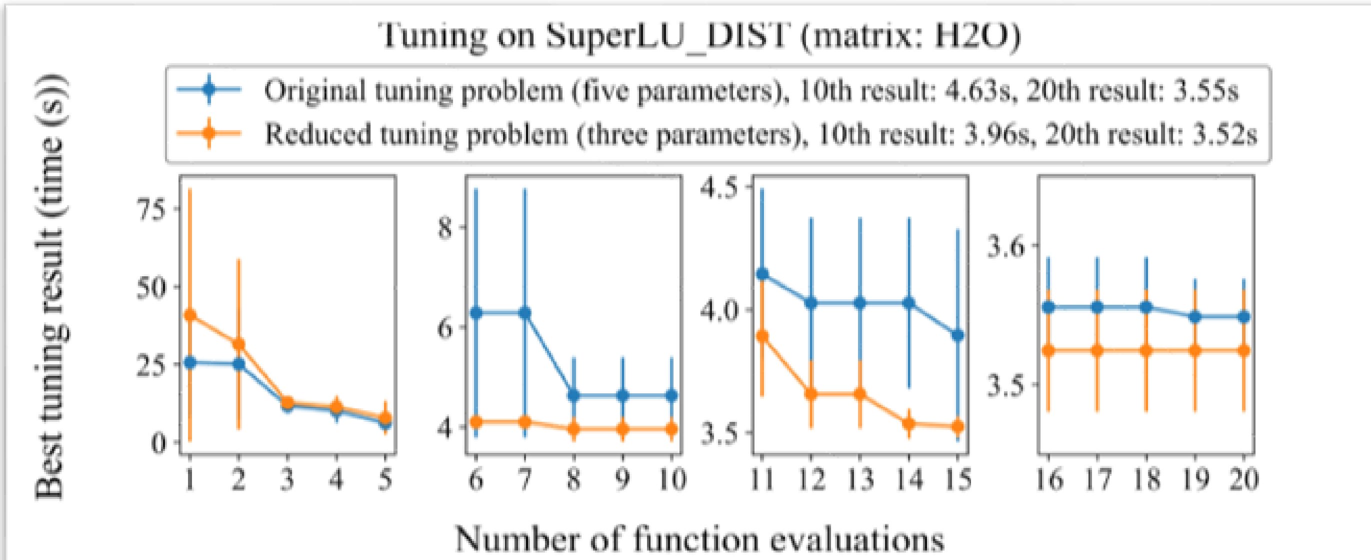
Example graphical representation on the web dashboard (matrix: Si5H12)
(thanks to Mohammad Zaeed and Tanzima Islam)

- We can reduce the tuning space based on the analysis

Note: analysis results are based on surrogate-based sampling, so the results can vary depending on the sampling setting

- Sobol analysis: https://en.wikipedia.org/wiki/Variance-based_sensitivity_analysis
- We internally use SALib for the sensitivity analysis computation: https://salib.readthedocs.io/en/latest/

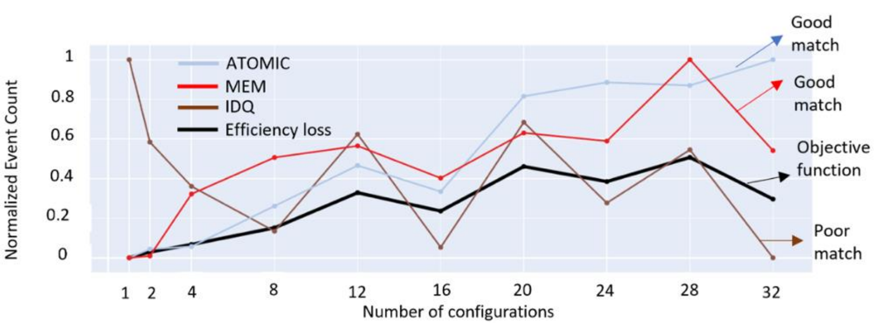
Feature 9: Crowd Tuning: Sensitivity Analysis



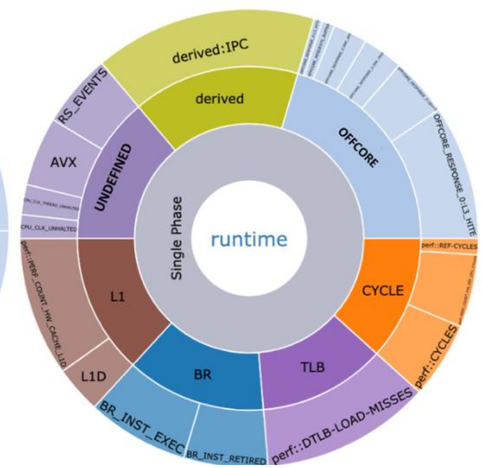
- SuperLU_DIST on four Haswell nodes in Cori
  - **Original tuning parameters: COLPERM, LOOKAHEAD, nprows, NSUP, NREL**
  - **Reduced tuning parameters: COLPERM, nprows, NSUP**

Feature 9: Crowd Tuning: Importance Analysis

- Incorporated Dashing(*)'s analysis/visualization in the history database
  - **Importance analysis on tuning parameters or hardware performance counters (and groups of them)**
  - **Interactive visualization on web (examples: PLASMA's DGEMM/DG at https://gptune.lbl.gov/repo)**
  - **Visualization for trend matching**



NIMROD (analysis on tuning parameters)



PLASMA's DGEMM (analysis on performance counters)

Analysis and Visualization of Important Performance Counters To Enhance Interpretability of Autotuner Output

Mohammad Zaeed[1], Tanzima Z. Islam[1], Younghyun Cho[3], Xiaoye Sherry Li[2], Hengrui Luo[2], Yang Liu[2]
[1]Texas State University, [2]Lawrence Berkeley National Laboratory, [3]University of California, Berkeley

(*) Islam et al., "Toward a programmable analysis and visualization framework for interactive performance analytics," IEEE ProTools, 2019