Targeted Adaptive Design

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Targeted Adaptive Design: Introduction

Targeted Adaptive Design (TAD) is a new data-driven model that aims at **efficiently** and **autonomously** locating control parameters that would yield a target output design within **specified tolerance**.

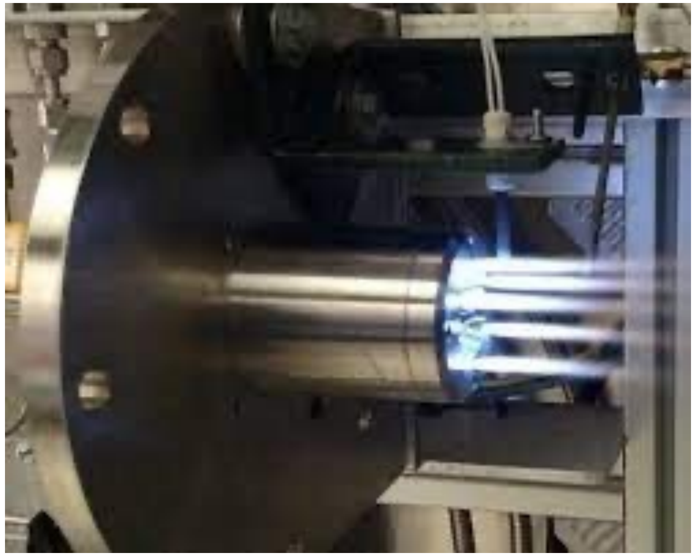
Motivation: Experimental design for advanced manufacturing

Example: Flame Spray Pyrolysis (FSP) optimization (Paulson et al,, 2020) with 6 control parameters that "result in desirable particle size distributions and simultaneously provide an understanding of the process itself

The upper and lower bounds for each processing variable are provided. Independent variables are green.

	lower	upper
TEOS concentration (wt%)	0.05	5
liquid flow rate (mL/min)	4	10
atomization O_2 flow rate (L/min)	6	12
pilot CH_4 flow rate (L/min)	2	4
pilot O_2 flow rate (L/min)	3	6
sheath O_2 flow rate (L/min)	15	25

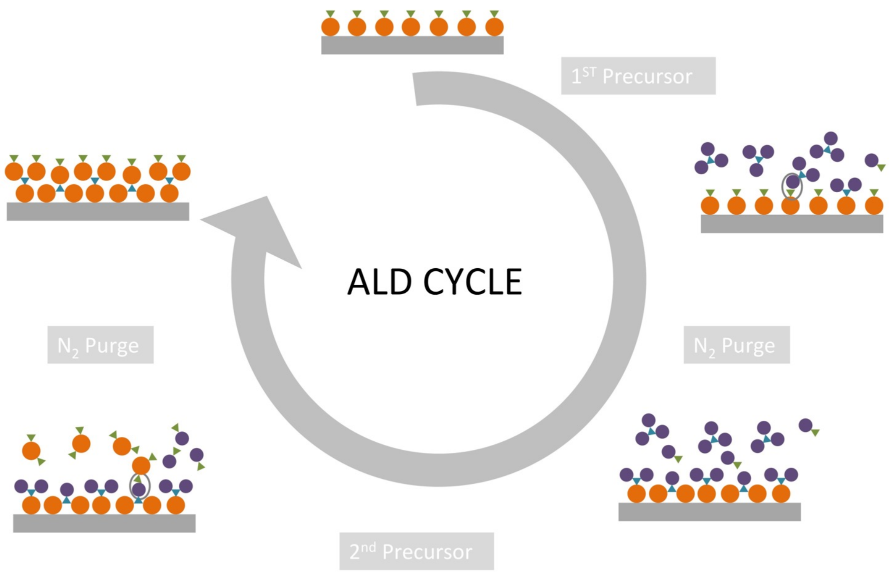
Paulson et al., Materials and Design 196 (2020) 108972 6



Argonne's FSP facility

Atomic Layer Deposition

- Advanced technique used for depositing thin films on a surface one atomic layer at a time



Source: ctechnano (https://ctechnano.com/coating-technologies/what-is-atomic-layer-deposition-ald/)

Each cycle is composed of four sequences:

- A dose period t_1 during which the substrate is exposed to precursor 1,
- A purge period t_2 during which there is no precursor exposure,
- A dose period t_3 during which the substrate is exposed to precursor 2,
- A final purge period t_4 during which there is no precursor exposure.

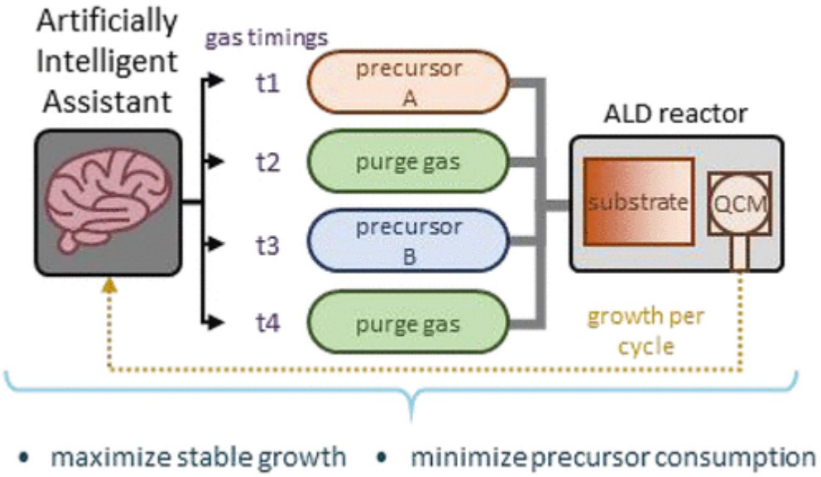
Applications: semiconductors, energy storage systems, biomedical devices etc.

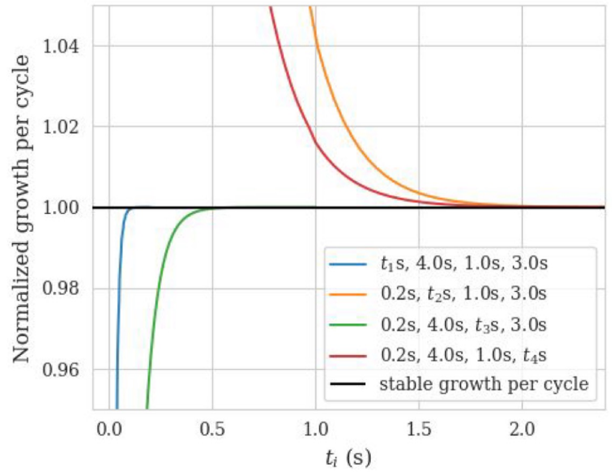
Atomic Layer Deposition (cont.)

- **GOAL:** Optimal Atomic Layer Deposition (ALD) film growth with minimal precursor consumption.

Several parameters can be controlled:

➢ Dose and purge times t_1, t_2, t_3, t_4

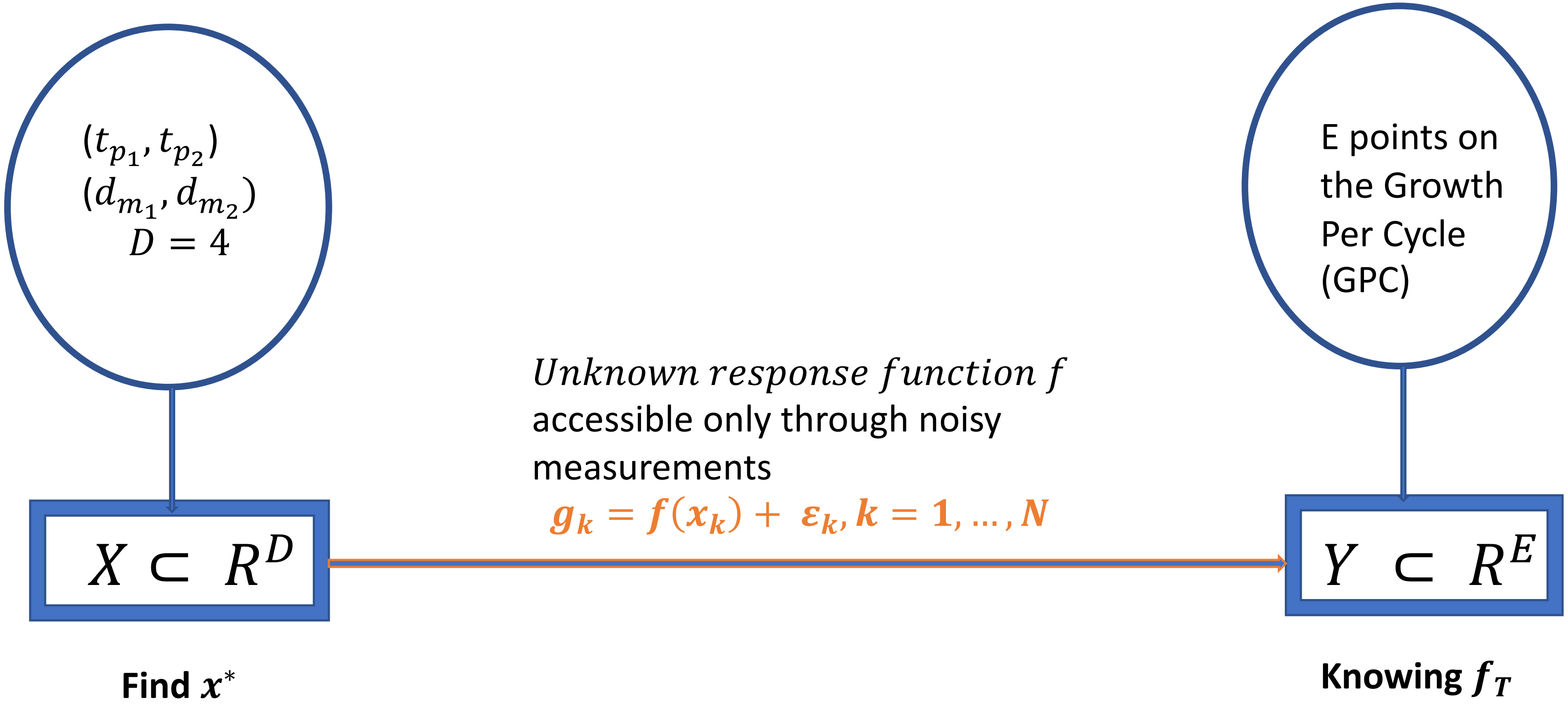




(Paulson et al., ACS Appl. Mater. Interfaces 2021, 13, 17022-17033).

➢ Temperature (T), site area (A), pressures (p_1, p_2), Molecular masses (M_1, M_2), the sticking probabilities (β_1, β_2) and the characteristic times for precursor evacuation (t_{p_1}, t_{p_2}) and the mass changes (d_{m_1}, d_{m_2}).

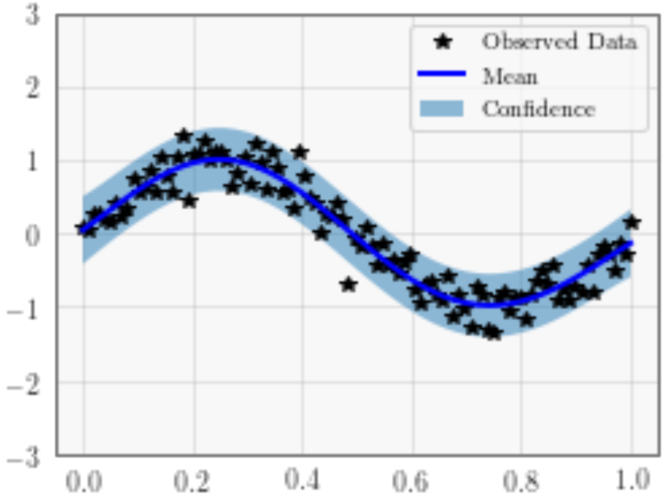
Problem set-up



TAD: (simplified) algorithm

- Place a Gaussian Process (GP is a probability distribution over possible functions)

prior on the unknown response function f (GP model is dynamically validated using chi—squared statistics)

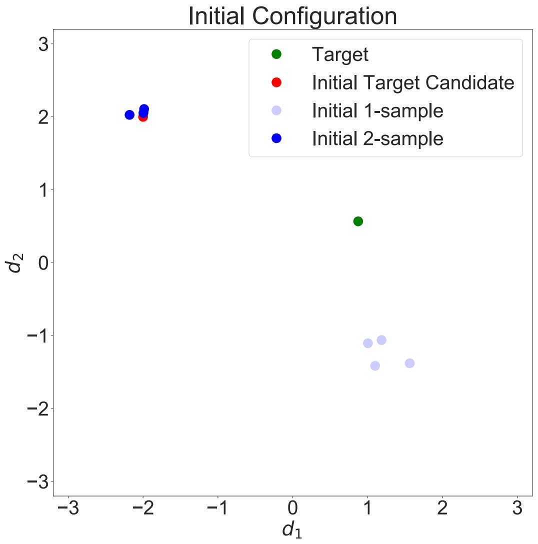


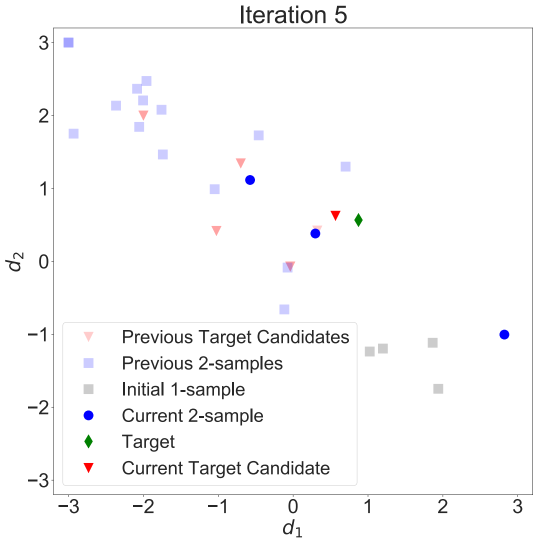
$f \sim GP(\mu_\theta, K_\theta)$, θ hyperparameters

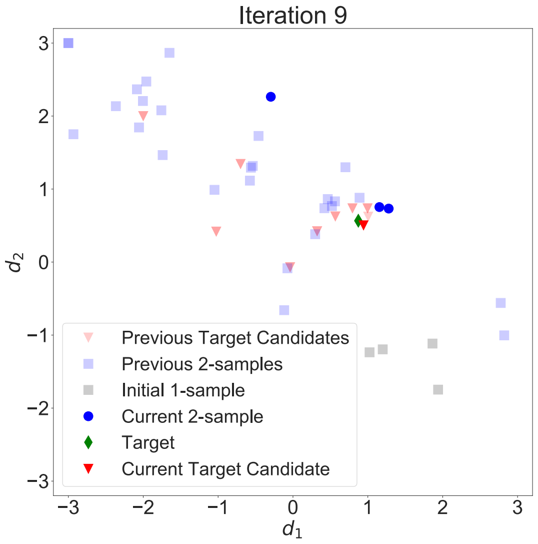
- Optimize an acquisition function to decide where to sample next,
- Acquire the points found at the previous step and update the GP model accordingly,
- Repeat until stopping criterion is met: (Success = found design within tolerance, Failure = Expected Shannon Information gain $< \varepsilon$)

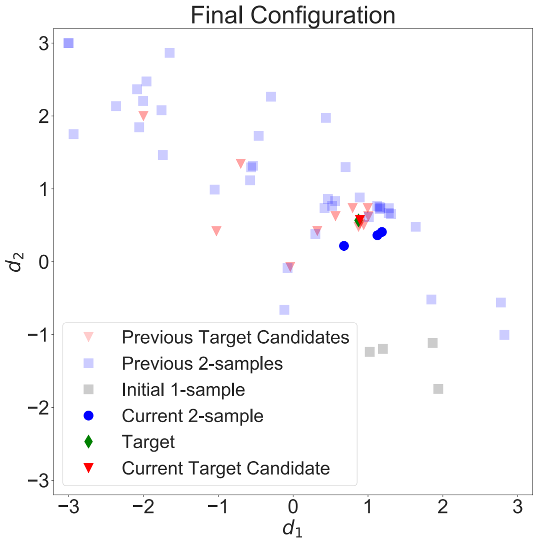
TAD

- TAD is a batch iterative algorithm.





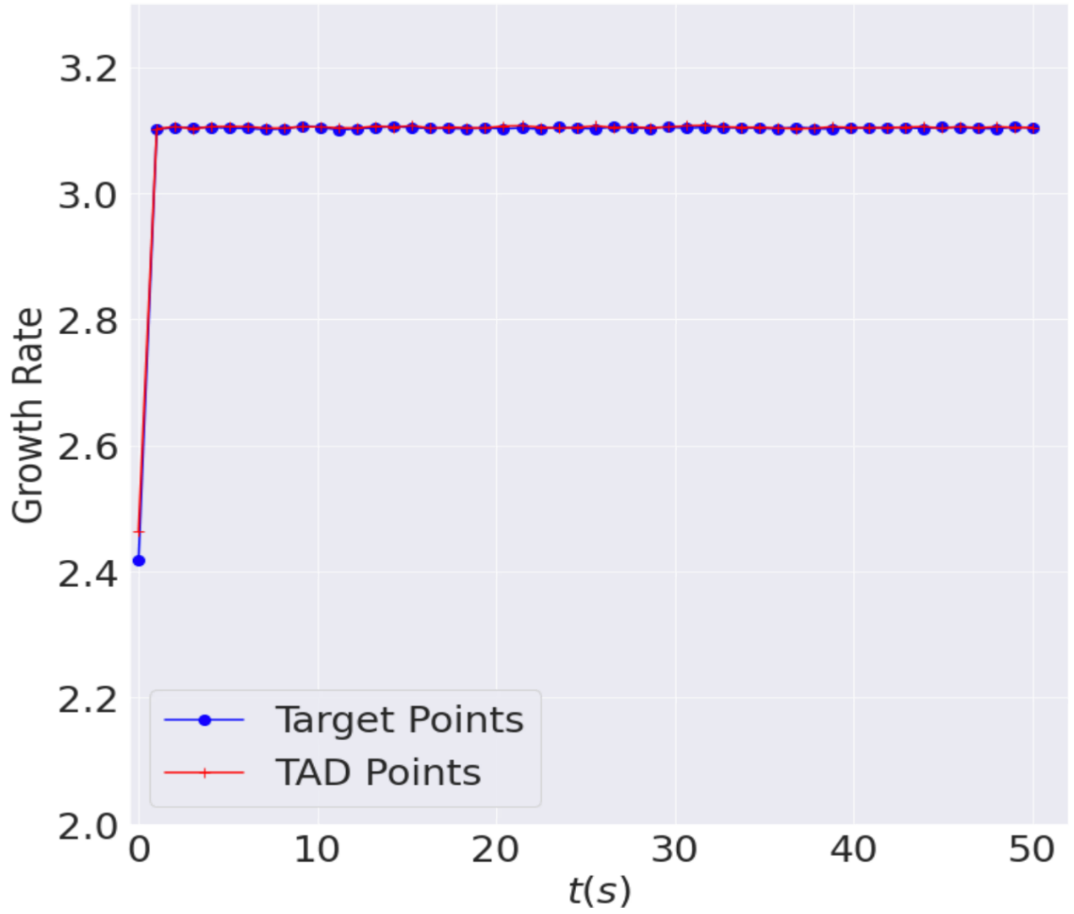




TAD at scale

- Gaussian processes involve the factorization of $\mathrm{E}N \times EN$ (N = data size, E = # of design objectives) covariance matrices which scales like E^3N^3 if using Cholesky for example,
- Solution: **Gpytorch** (a highly efficient and modular implementation of GP implemented in Pytorch and which allows to train GPs with millions of data points.)
- On the scalability of TAD on SambaNova (ANL LDRD): We are applying TAD to ALD and evaluating its performance on GPU (ThetaGPU) and on SambaNova.

Test case: 50 points on the GPC, 4 control parameters



Target GPC: $t_1 = t_2 = t_3 = t_4 = 0.25s$

$T = 473\ K, A = 22.5^{-20}m^2, p_1 = p_2 = 26.66\ Pa,$

$M_1 = 72AMU, M_2 = 18AMU, \beta_1 = 1^{-3}, \beta_2 = 1^{-4},$

$$\boldsymbol{t_{p_1} = 0.2s, t_{p_2} = 0.3s,}$$
$$\boldsymbol{d_{m_1} = 0.8\ ngcm^{-2}, d_{m_2} = 0.5\ ngcm^{-2}}$$

TAD solution: $\boldsymbol{t_{p_1} = 0.2544s, t_{p_2} = 0.3091s,}$
$\boldsymbol{d_{m_1} = 0.5864\ ngcm^{-2}, d_{m_2} = 0.6126\ ngcm^{-2}}$

Initial sample size: **20**, # of new points per iteration: **10+1**, tolerance: 10%

Convergence after **2** iterations (**42** points total sampled, matrix size: **50x42**)

GP fitting time: **4.3s**, TAD optimization time: **15.8s**

Conclusions and outlook

- TAD is a new, efficient and scalable algorithm specifically well-suited for design problems,
- It incorporates a new acquisition function that balances well the exploration/exploitation tradeoff, and a dynamical model validation.
- Ongoing/future work:
  - TADxALD at scale (LDRD, joint work with N. Paulson (DSL/AMD))
  - TADxconcrete_mixing (collaboration with C. Tavares & K. Skillen, Texas A&M)

THANK YOU! ANY QUESTIONS?