Surrogates:

Revised and updated previously identified dimensions and characteristics of surrogates:

- **Algorithmic dimension**: concerned with the machine learning model used and the resulting architecture and its properties.

    * *Machine learning model*: most work to date in building surrogates uses random forests[4], Gaussian Processes[5], CNN[14], FCN[20], RNN[20], or other machine learning models [6,7]. Non- Neural Network models have limited ability to model high-dimensional inputs/outputs. Dimensionality reduction techniques can enable higher dimensional inputs/outputs but the improvement is limited [21,22]. Thus, Neural Network models are more suitable for processing natural n-dimensional signals. However, most existing deep active learning methods are concerned with classification tasks while Neural surrogates are generally concerned with regression tasks.

    * *Machine Learning Architecture*: finding the "correct" architecture is instrumental in the successful learning of surrogate models. For example, CNN priors inherently rely on their architectures, one has to find an architecture that gives the suitable prior of a given problem. However, required optimal architecture is likely to change when training data changes. Therefore, it is important to have a variable architecture that can adjust with associated uncertainty

    * *Variability of the architecture*: Most surrogates used in scientific workflow use a fixed architecture [4-7]. However, a recent paper [14] successfully used NAS (Neural Architecture Search) in order to infer the architecture of the CNN-based neural surrogate. Further work needs to be done to use NAS with other NN models.

- **Data dimension**: is a sub-dimension of the algorithmic dimension. Concerned with the generation, labeling and selection of the data used to train the ML model.

    * *Data set generation and labeling:* in supervised (sequential) learning, the labeled data set is given beforehand and learning is performed afterwards (offline)[4]. In concurrent machine learning, the data set is generated and labeled as model training proceeds (Online) [8]. In active learning, we are given the unlabeled data, and we decide which ones should be labeled during the training process[9].

    * *Data selection method:* Most surrogates models require human intervention for the selection and adjustment of training data [4-7]. However, an active approach to surrogates learning that enables automatic training data selection has emerged in GP surrogates[15].

    * *Data Volume*: Since the training data generation typically involves numerical solutions of the underlying micro-scale model, a process that is often quite expensive, learning an efficient surrogate is a small data problem. Datasets vary in size from of a few hundred[18] or a few thousand[16,17,19] individual simulations. The dataset that one

uses to construct the model should be a good representation of all the practical situations that the model is intended for.

- **Functionality Dimension**: concerned with the functionality of the surrogate and the link between ML and HPC:

  * *Link between ML and HPC*: HPCforML uses HPC to execute and enhance ML performance, or uses HPC simulations to train ML algorithms, which are then used to understand experimental data or simulations. MLforHPC uses ML to enhance HPC applications and systems [10]. HPC- surrogate conjunction can be used to 1) train surrogates [23], 2) replace simulation [25] or a component of it [24] and 3) to guide computations [26].

- **Problem Dimension**: concerned with the algorithmic area and the dimentionality of the problems.

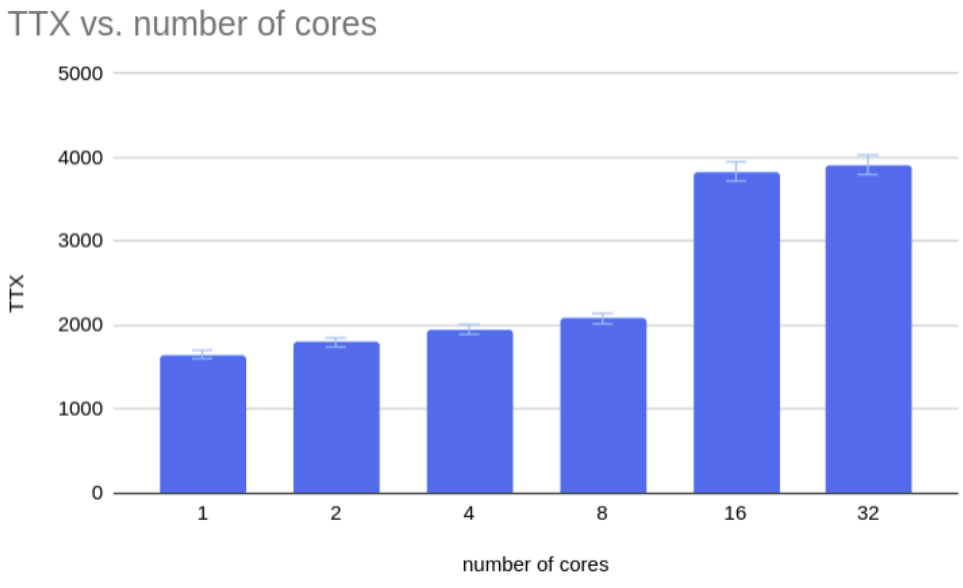
  * *Dimentionality of the problem*: as the dimensionality grows, the complexity (or computational cost) grows exponentially.

  * *Algorithmic area*: The scientific problem the surrogate is investigating. For example: partial differential equations, particle dynamics.

RCT:

See ss_updated_1.py, ss_updated.py and ws_updated.py for the code.

Weak scaling:
Performed 3 experiments each consisting of a varying number of pipelines. Each pipeline contains 12 stages each containing 1 task(100s stress-ng). The number of pipelines = 4* the number of cores. The results show a gradual increase in TTX followed by a more steep increase when going from 8 to 16 cores. These results are consistent among the three experiments. The reason for the sudden steep increase in TTX at 16 cores might be the increased overhead when going from 32 to 64 pipelines.



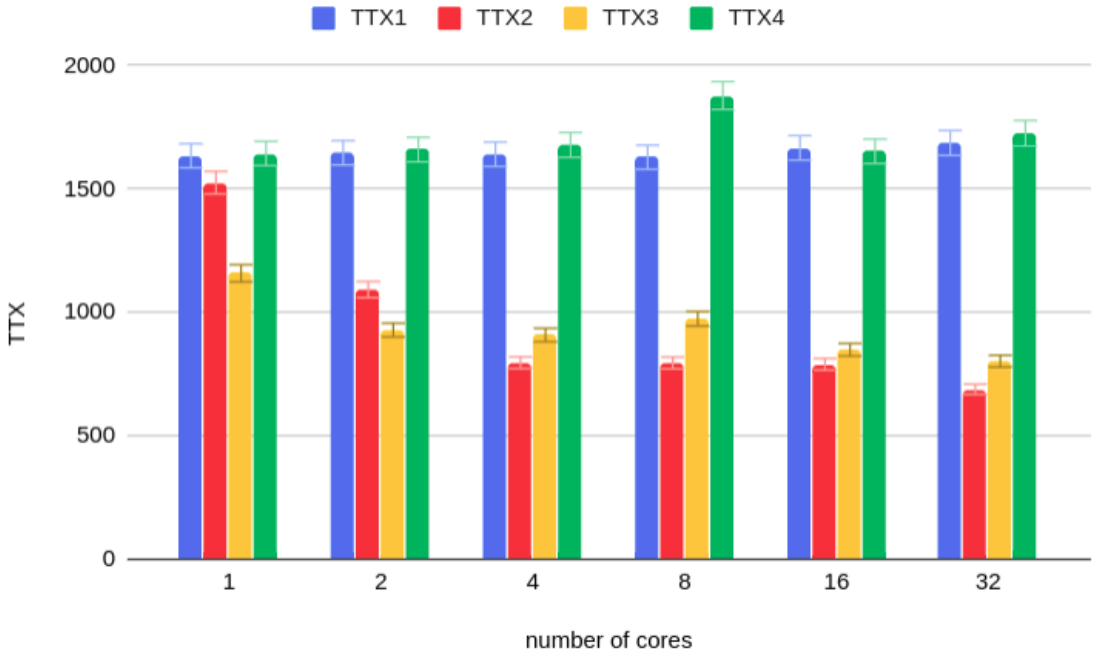
Strong scaling:
Performed 4 experiments each repeated 3 times. The structure and executables are as follows:

Experiment Number	Number of pipelines	stages/pipeline	Executable
1	10	12	100-second stress
2	30	4	100-second stress
3	30	4	Generates random numbers for 100 seconds
4	10	12	Generates random numbers for 100 seconds

*each stage consists of 1 task

I expected the time needed to execute an application to decrease in half(almost) with the doubling of the number of cores.

In experiments 1 and 4, TTX remained the same despite the increase in the number of cores. This is different from my expectation. Since I use two different executables in the 2 experiments, it's unlikely that a problem with the executables is the reason for the observed result. The results suggest that no significant parallization was happening with the increase in the number of cores; ie, maximal parallization is happening with only 1 core. This is unexpected since each core has only 1 thread. To enable more parallization, I increased the number of pipelines while keeping the total number of tasks the same as in experiment 1. The results of experiments 2 and 3 were more consistent with my expectations. However, the decrease in TTX is not as steep as expected. This might be explained by the increased overhead due to having multiple cores.



Next Semester:

I will work on a project instead of a thesis.

Resources:

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