Parallel-in-time methods with ML

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Overview

Motivation

Differential equations

- numerous scientific and engineering problems are described by time-dependent differential equations
- ODEs and PDEs
- many different numerical methods exist for solving them [1]

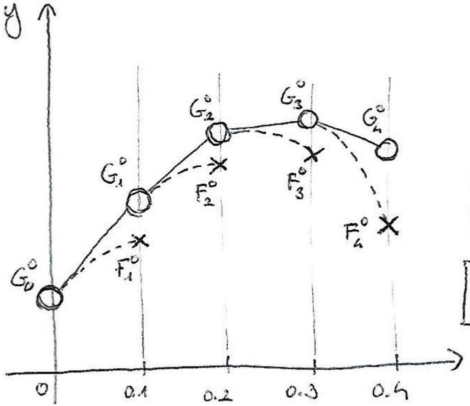
Parallelism

- traditionally, parallelised across the system or across space [2]
- good weak scaling, limited strong scaling
- but for some problems only wall time matters (e.g. stock trading)
- need to exploit parallelism better to reduce wall clock time

Parallel-in-time methods

- solution parallelised across the time steps
- more CPU time, less wall clock time
- parareal algorithm [3] for solving IVPs
- relies on two operators, coarse G and fine F
- for every iteration, G executed serially, F in parallel
- G must be fast but preferably also accurate enough

Parareal algorithm



$$y'(t) = f(y(t), t)$$
$$y(t_0) = y_0$$
$$t_0 \leq t \leq T$$

$$G_n^k = G(y_n^k, t_n, t_{n+1})$$
$$F_n^k = F(y_n^k, t_n, t_{n+1})$$

$$\boxed{y_{n+1}^k = G_n^k + \underbrace{F_n^{k-1} - G_n^{k-1}}_{\text{correction term}}}$$

Hypotheses

Hypotheses

1. an ML (regression) model can be trained and used as G to solve differential equations in a parareal framework
2. for some problems, the ML model based G operator is better than traditional coarse operators in terms of performance and accuracy
3. for some problems, the ML accelerated parareal framework achieves shorter wall time than a conventional parareal algorithm or a state-of-the-art traditional solver using the same number of CPU cores
   a. training time ignored
   b. training time taken into account

Related work

Related work

- neural network for solving time-dependent differential equations [4]
- neural network to approximate the gradients of high-dimensional PDEs [5]
- physics informed neural network (PINN) for solving PDEs [6] [7] [8]
- parareal solver using a PINN as F [9]

Challenges

Challenges

- numerical analysis is a complex field
- fast moving area of research
- many potential avenues (PDE solving methods, model training, tech stack)
- aiming high

Plan

Implementation

- develop a simple parareal framework
  - already implemented first version in C with POSIX threads
- construct an ML model (PINN vs standard models)
- train the model using targets provided either by G or F
- automatise the model training as part of the framework
- use the trained model for inference as G
- extend the framework to discretise PDEs or handle PDEs directly through the model

Problem iterations

- ODE (Lotka-Volterra)
- simple PDE (2D diffusion)
- high-dimensional PDE (Black-Scholes)

Performance

- compare the ML version of G to traditional ODE solvers of similar accuracy
- compare the performance of the parareal framework to traditional ODE and PDE solvers and analyse the impact of the model training on performance
- try different ML models (linear regression, ANN, RNN, etc.)
- take advantage of Cirrus' new GPUs

Tech stack

- C/C++ faster than Python but most scientific Python libraries are just wrappers on top of C bindings
- Python better suited for ML and numerical solver libraries are easier to use
- mpi4py [10] for distributed computing
- scikit-learn [11] and keras [12] for ML
- FEniCS [13] (finite element) and FiPy [14] (finite volume) to compare performance against

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