An Investigation into Parareal

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Problem Statement

We would like to numerically solve the autonomous ordinary differential equation:

$$\begin{cases} u'(t) = f(t, u), & t \in [t_0, t_f] \\ u(t_0) = u_0 \end{cases}$$

where $f: \mathbb{R}^d \to \mathbb{R}^d$ and $u: \mathbb{R} \to \mathbb{R}^d$.

Framing this in a HPC context, how can we solve the above while taking advantage of massively parallel hardware?

Forward and Backward Euler:

$$u_{n+1} = u_n + hf(t, u_n), u_n + hf(t, u_{n+1})$$

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Linear Multistep Methods

$$\sum_{k} \alpha_{k} y_{n+k} = h \sum_{k} \beta_{k} f(t_{n+k}, y_{n+k})$$

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Runge Kutta Methods

Forward and Backward Euler:

$$u_{n+1} = u_n + hf(t, u_n), u_n + hf(t, u_{n+1})$$

Linear Multistep Methods

$$\sum_{k} \alpha_{k} y_{n+k} = h \sum_{k} \beta_{k} f(t_{n+k}, y_{n+k})$$

- Runge Kutta Methods
- Etc.

Parallel Techniques

Problem!

Most of the previous methods are iterative, depending on the previously computed values.

Not embarrassingly parallel... We have to get creative.

Parallel-In-Time

One technique is to parallelize the problem across time, i.e. split $[t_0, t_f]$ into slices $[t_n, t_{n+1}]$ and in parallel solve each slice.

Iteration Dependence

But since each slice depends on the previous, how can we chain together these individual solutions to each slice?

Parareal

Predictor-Corrector

What if we were to predict the portions that $[t_n, t_{n+1}]$ are dependent on with a cheap course operator, and then correct with a fine operator!

Yes!

Parareal

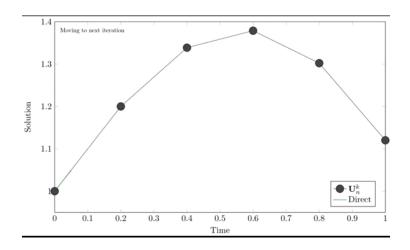
Let $\mathcal G$ be a course and inexpensive operator, and let $\mathcal F$ be a fine operator of high order. Then Parareal iteration is:

$$\lambda_{n+1}^{k+1} = \mathcal{G}(t_{n+1}, t_n, \lambda_n^{k+1}) + \mathcal{F}(t_{n+1}, t_n, \lambda_n^{k}) - \mathcal{G}(t_{n+1}, t_n, \lambda_n^{k})$$

Parallel Potential

Notice! The \mathcal{F} term depends only on the previous solutions, which means it can be computed in parallel for each k step. Furthermore, $\mathcal{G}(\lambda_n^k)$ satisfies the FSAL property!

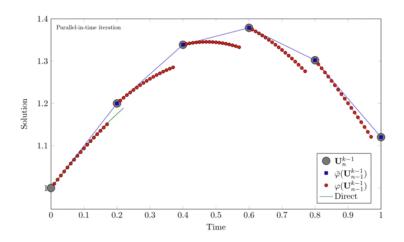
Parareal: Visual Example



Full beautiful animation found on wikipedia's Parareal page.



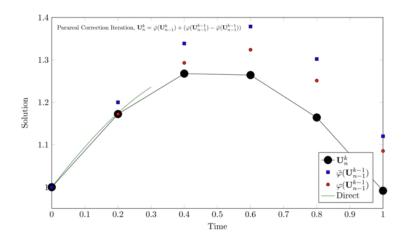
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Pseudocode

```
Require: y_0 and course and fine solvers \mathcal{G}, \mathcal{F}.
y_c \leftarrow \mathcal{G}(t_f, t_0, y_0).
                              Coarsely approximate solution
y \leftarrow y_c.
while iter < \max_{i} ter \&\& not converged do
     for n=0 \rightarrow P do
                                                   ▶ Parallel capable
         y_f(n) = \mathcal{F}(t_{n+1}, t_n, y(n)).
         \delta y(n) = y_f(n) - y_c(n).
                                      end for
     for n=0 \rightarrow P do
         y_c(n) = \mathcal{G}(t_{n+1}, t_n, v(n)).
                                                             ▶ Predict
         v(n) = v_c(n) + \delta v(n).
                                                             Correct
     end for
end while
```

Parallel Pseudocode

```
Require: y_0 and course and fine solvers \mathcal{G}, \mathcal{F}.
y_c \leftarrow \mathcal{G}(t_f, t_0, y_0).
                             Coarsely approximate solution
y \leftarrow y_c.
while iter < max_iter && not converged do
    #pragma omp parallel for
    for n=0 \rightarrow P do
        y_f(n) = \mathcal{F}(t_{n+1}, t_n, y(n)).
        \delta v(n) = v_f(n) - v_c(n).
                                     end for
    for n=0 \rightarrow P do
        y_c(n) = \mathcal{G}(t_{n+1}, t_n, y(n)).
                                                            ▶ Predict
        y(n) = y_c(n) + \delta y(n).
                                                           Correct.
    end for
end while
```

Speedup Analysis

Suppose we have P processors, and suppose our fine method takes T_f time, T_g for the course method. Furthermore, assume that our Parareal iteration needs k steps. Then the speedup it provides is:

$$S = \frac{PT_f}{PT_g + k(PT_g + T_f)} = \frac{1}{\frac{T_g}{T_f} + k(\frac{T_g}{T_f} + \frac{1}{P})} = \frac{1}{\frac{T_g}{T_f}(1 + k) + \frac{k}{P}}$$

Note:

$$\lim_{P\to\infty}\frac{1}{\frac{T_g}{T_f}(1+k)+\frac{k}{P}}=\frac{T_f}{T_g(1+k)}$$

No Free Lunch

$$S_{\infty} = \frac{T_f}{T_g(1+k)}$$

This tells us something very important, we want the ratio T_f/T_g to be as large as possible, and we want k to be as small as possible.

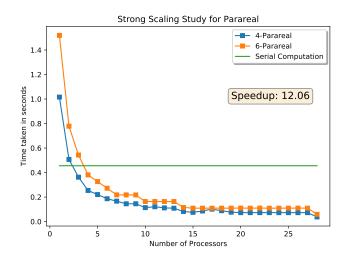
Theorem

The parareal method has order of accuracy mk, where k-1 is the number of parareal iterations made and m is the order of \mathcal{G} , assuming \mathcal{F} is close to truth. (Bal)

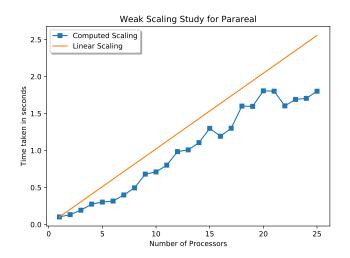
Therefore, we have this uncomfortable optimization problem. We want k small for speedup, but large for order. If we make m large instead, then the ratio T_f/T_g becomes smaller...



Strong Scaling



Weak Scaling



Improvements | Pipelined Parareal

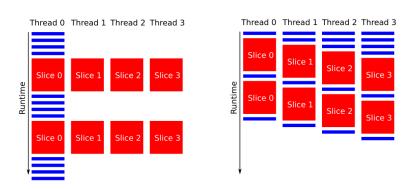


Figure borrowed from Ruprecht's Implementing Parareal.

Pipelined Parareal Pseudocode

It's a bit too complicated to present in a slide, but the general idea is to begin the omp parallel statement at the beginning and then pretend like were in a MPI enviornment.

General Idea

Thread p processes the new iteration at p+1. MPI communication is mimicked with locks, and done in place.