Parareal Methods

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Outline

- The parareal algorithm
- Properties: Convergence, Stability, and Parameters
- Matlab example
- Conclusion: Advantages, disadvantages, and survey of usage in literature

Overview

- Proposed by Lions, Maday, Turinici in 2001
- Parareal = "Parallel in time" ODE solver
- Low order accurate solution obtained via serial computation to a final time
  - e.g foreward Euler
- Corrections to low order solution done in parallel
  - e.g. on a finer temporal grid

Notation and Problem Statement

- $u' = f(t,u)$ on coarse mesh $t^n = n\Delta t$. n = 0, 1, ..., N
  IC $u^0 = u(t^0)$
- Three flavors of solution operator
  - Analytic: $u(t^{n+1}) = g(t^n, u(t^n))$
  - Numerical, coarse with order m: $u^{n+1} = g_{\Delta t}(t^n, u^n)$
  - Numerical, fine: $u^{n+1} = g_{\text{fine}}(t^n, u^n)$
- One might choose the fine solution operator such that $\Delta t/100$, or use a method with an order of accuracy higher than m.
- $\delta g^n(u) = g_{\text{fine}}(t^n, u) - g_{\Delta t}(t^n, u)$
- Introduce a correction iteration label u_k^{n+1}, where $k = 1, 2, \ldots$. k will denote the number of refinements, and $u_1^{n+1} = g_{\Delta t}(t^n, u^n)$.

Algorithm

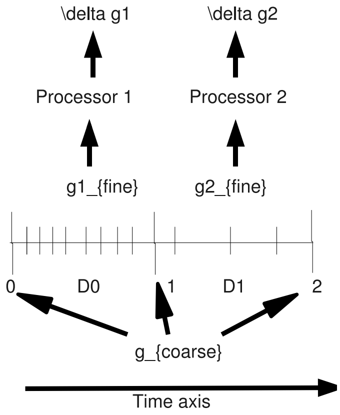
After choosing a temporal discretization and schemes $g_{\Delta t}$ and g_{fine}, the following iterative procedure comprises the parareal algorithm

1. compute $u_1^{n+1} = g_{\Delta t}(t^n, u^n)$ in serial
2. compute the corrections $\delta g^n(u_1^n) = g_{\text{fine}}(t^n, u_1^n) - g_{\Delta t}(t^n, u_1^n)$ in parallel
3. add the prediction and correction terms as $u_2^{n+1} = g_{\Delta t}(t^n, u_2^n) + \delta g^n(u_1^n)$
4. repeat steps 2 and 3, incrementing the iteration label and using $u_{k+1}^0 = u^0$ as the initial condition.

Or more compactly

$$u_{k+1}^{n+1} = g_{\Delta t}(t^n, u_{k+1}^n) + [g_{\text{fine}}(t^n, u_k^n) - g_{\Delta t}(t^n, u_k^n)] \qquad k = 1, 2, \ldots$$

A Time Domain Decomposition



Comments on the algorithm

$$u_{k+1}^{n+1} = g_{\Delta t}(t^n, u_{k+1}^n) + [g_{\text{fine}}(t^n, u_k^n) - g_{\Delta t}(t^n, u_k^n)]$$

- Optimally we will have N processors.
- Example: if $k = 1$ we recover the order m scheme. if, say k=3, we have an order 3m scheme requiring 3 coarse computations in serial, and 2 correction calculations in parallel.
- as $k \longrightarrow N$ the parareal algorithm gives $u_{k+1}^n = u_k^n$, producing a solution with accuracy of g_{fine}.
- One would like to take large steps with $g_{\Delta t}$. Choosing an appropriate implicit method is a popular choice.

Choices (to be discussed throughout the talk) must be made for k, Δt, methods for g_{fine} and $g_{\Delta t}$, and the number of processors P.

Example: model equation

Our problem is $u' = \lambda u$ s.t. $\lambda < 0$ and $u^0 = 1$.

Let the fine solution operator be exact $g_{\mathrm{fine}} = g$ and the coarse operator be a forward Euler scheme. Define $z = \lambda \Delta t$, thus

$$g_{\mathrm{fine}} = e^z$$
$$g_{\Delta t} = 1 + z \Rightarrow u_1^n = (1+z)^n = e^z + O(\Delta t)$$
$$\delta g(u) = [e^z - (1+z)]\, u$$

For the $k = 2$ iteration we have...

$u_2^0 = 1$

$u_2^1 = (1+z) + \delta g(u_1^0) = e^z$ EXACT!

$u_2^2 = (1+z)^2 + (1+z)\delta g(u_1^0) + \delta g(u_1^1) = e^{2z} + O((\Delta t)^2)$

Example: model equation

$$
\begin{aligned}
u_2^{n+1} =& (1+z)^{n+1} + \sum_{j=0}^{n} (1+z)^{n-j} \delta g(u_1^j) \\
=& (1+z)^{n+1} + \sum_{j=0}^{n} (1+z)^{n-j} \left[e^z - (1+z) \right] (1+z)^j \\
=& (1+z)^{n+1} + (n+1)(1+z)^n \left[e^z - (1+z) \right] \\
=& e^{(n+1)z} + O((\Delta t)^2)
\end{aligned}
$$

- From our first order FE, we now have a second order parareal method! This example is representative of the general theory...

Theory: Convergence, Stability, and Parameters

Assumptions

Assume the coarse operator $g_{\Delta t}$ is order m and Lipschitz:

$$|g_{\Delta t}(t^n, u) - g_{\Delta t}(t^n, v)| \leq (1 + L\Delta t)|u - v| \quad \forall t \in (0, t^N)$$
$$|u(t^N) - u_1^N| \leq C\,(\Delta t)^m\,|u_0|$$

It is also assumed that the function u remains bounded on $(0, t^N)$.

Convergence

Assume the fine solution operator is sufficiently accurate approximation to the analytic operator so that we may replace $g_{\text{fine}} \to g$

Theorem: The order of accuracy of the parareal method with coarse solution operator $g_{\Delta t}$ and fine operator g is mk. (G. Bal www.columbia.edu/ gb2030)

proof: By induction

k=1: This is just the order m coarse operator.

Assume for k: $|u(t^N) - u_k^N| \leq C\,(\Delta t)^{mk}\,|u_0|$

now show k $\Rightarrow$ k+1:

Convergence

k $\Rightarrow$ k+1:

$$
\begin{aligned}
|u(t^N) - u_{k+1}^N| &= |g(u(t^{N-1})) - g_{\Delta t}(u_{k+1}^{N-1}) - \delta g(u_k^{N-1})| \\
&= |g_{\Delta t}(u(t^{N-1})) - g_{\Delta t}(u_{k+1}^{N-1}) - \delta g(u_k^{N-1}) + \delta g(u(t^{N-1}))| \\
&\leq |g_{\Delta t}(u(t^{N-1})) - g_{\Delta t}(u_{k+1}^{N-1})| + |\delta g(u_k^{N-1}) - \delta g(u(t^{N-1}))| \\
&\leq (1 + C\Delta t)|u(t^{N-1}) - u_{k+1}^{N-1}| + C(\Delta t)^{m+1}|u_k^{N-1} - u(t^{N-1})| \\
&\leq (1 + C\Delta t)|u(t^{N-1}) - u_{k+1}^{N-1}| + C(\Delta t)^{m(k+1)+1}|u_0|
\end{aligned}
$$

$$\therefore |u(t^N) - u_{k+1}^N| \leq C\,(\Delta t)^{m(k+1)}\,|u_0|$$

Stability

- Parareal methods prescribe a means for combining ODE solvers. Thus a study of the stability region requires specifying $g_{\Delta t}$ and g_{fine}. Consider $u' = \lambda u$
- Let $g_{\mathrm{fine}}(t^n, u^n) = \bar{g}_{\mathrm{fine}} u^n$ and $g_{\Delta \mathrm{t}}(t^n, u^n) = \bar{g}_{\Delta \mathrm{t}} u^n$
- As shown in *Stability of the Parareal Algorithm* by Staff et al. the parareal method becomes

$$u_k^n = \left(\sum_{j=0}^{k} \binom{n}{j} \left(\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}\right)^j \bar{g}_{\Delta \mathrm{t}}^{n-j} \right) u_0 = H(\bar{g}_{\Delta \mathrm{t}}, \bar{g}_{\mathrm{fine}}, n, k, \lambda) u_0$$

- Stability $\Rightarrow \max_{\forall n,k} |H| \leq 1$

Stability

- The authors go on to show that when $\lambda \leq 0$ and real,

$$|H| \leq \sum_{j=0}^{n} \binom{n}{j} |\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}|^j |\bar{g}_{\Delta \mathrm{t}}|^{n-j}$$
$$= (|\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}| + |\bar{g}_{\Delta \mathrm{t}}|)^n \leq 1$$
$$\Rightarrow |\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}| + |\bar{g}_{\Delta \mathrm{t}}| \leq 1$$

- The conditions are:
  1. $|\bar{g}_{\mathrm{fine}}| \leq 1 \rightarrow$ this is the usual stability requirement.
  2. $|\bar{g}_{\mathrm{fine}} - 2\bar{g}_{\Delta \mathrm{t}}| \leq 1$
- Example: $\bar{g}_{\Delta t} = (1 - \lambda \Delta t)^{-1}$ and $\bar{g}_{\mathrm{fine}} = (1 + \lambda \frac{\Delta t}{10})^{10}$

Stability

- Parareal methods work best when there is (numerical or analytic) dissipation. Consider the k^{th} term in H $\binom{n}{k}|\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}|^k |\bar{g}_{\Delta \mathrm{t}}|^{n-k}$.
- For $k << n$, $\binom{n}{k} < n^k$ is a good bound.
- Thus a desirable property would be $n^k|\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}|^k |\bar{g}_{\Delta \mathrm{t}}|^{n-k} \leq 1$
- Terms 2 and 3 must compensate for the presence of n^k. We must have
    1. $|\bar{g}_{\Delta \mathrm{t}}| \leq (1 + c\Delta t)e^{-\gamma[\min(|\lambda \Delta t|^{\beta},1)]}$
    2. $|\bar{g}_{\mathrm{fine}} - \bar{g}_{\Delta \mathrm{t}}| \leq c\min(|\lambda \Delta t|^{m+1}, 1)$
- $\gamma > 0$ and $\beta \geq 1$ chosen to satisfy $e^{-\gamma n} n^k \leq 1$ and $|\lambda \Delta t|^{k(m+1)} n^k e^{-n\gamma|\lambda \Delta t|^{\beta}} \leq 1$

Stability

Guillaume Bal: "The parareal algorithm [...] may generate instabilities. "

2 stage, 3 third order RK-Radau method (A-stable)

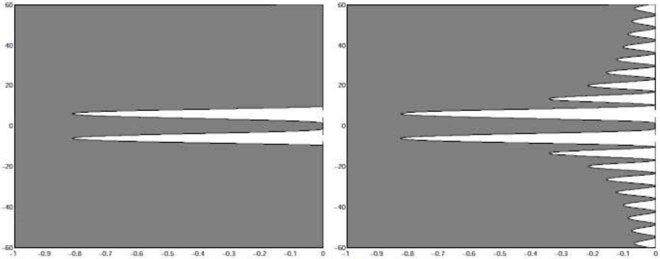


Fig. 3. Stability plots using Radau3 for both $\mathcal{G}_{\Delta T}$ and $\mathcal{F}_{\Delta T}$. The x-axis is $\mathrm{Re}(\mu \Delta T)$ and the y-axis is $\mathrm{Im}(\mu \Delta T)$. The dark regions represent the regions in the complex plane where (6) is satisfied. Here, $N = 1000$, and $s = 10$ (left) and $s = 1000$ (right).

Choosing the parameters wisely

In Bal *Parallelization In Time of ODEs*, the author attempts to optimize

- Speedup S = (full fine resolution)/ (parallel algorithm)
- Efficiency E = S/P, where P = processors. Best case E = 1

Assuming an order 1 course and fine solution operator, the main points are as follows

- $E \leq (k-1)^{-1}$
- S can be unbounded at the expense of E

Proposes a "mult-level" parareal method to improve S and E (essentially applies k=2 case hierarchically).

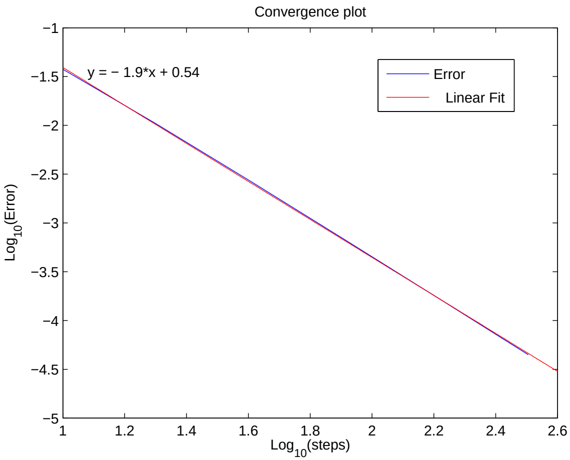
Matlab Example

Problem and Code

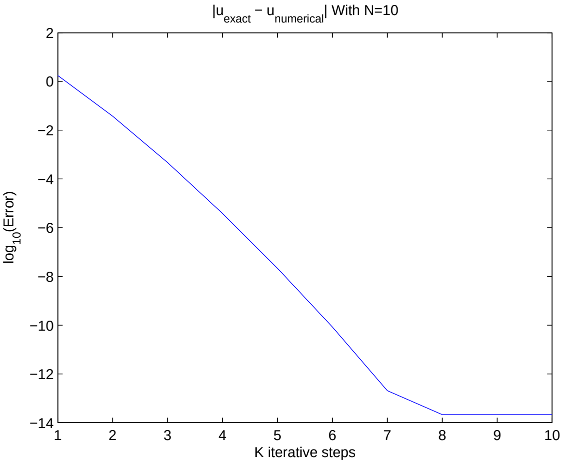
Consider the model problem, with a BE coarse solution operator and the exact operator use as the fine operator. The Matlab code is

```
lambda = -1; TF=1;  nsteps=2e3;
h=TF/nsteps; dts = 0.0:h:TF;
y=100;

solution=zeros(1,nsteps+1);
correction = zeros(1,nsteps+1);
solution(1,1)=y;
coarse = (1-h*lambda)^-1;
fine = exp(lambda*h);
corrector = fine - coarse;

tic
for k=1:10 %number of refinements
    for ii=1:nsteps %number of coarse steps
        y = coarse*y + correction(ii);
        solution(1,ii+1)=y;    %save solution
    end
    %compute corrections at each coarse step
    correction = corrector*solution;
    y=solution(1);
    error(k) = solution(end)-100*exp(lambda*TF)
end
toc
```

Δt convergence for K=2



k convergence



Conclusion

What have other people used parareal for?

- Martin Gander: Fourier transformed heat and wave equations. For the latter an exact solution operator was used in place of a fine operator.
- Guillaume Bal: Exponential funcion, harmonic oscillator, Brownian motion. Typical speedup and efficiency

we obtain for $M = 1$ that

$$dT = 7.21\,10^{-9}, \quad \Delta T = 9.67\,10^{-5}, \quad P = 10341, \quad S = 3987, \quad E = 0.40,$$

and for $M = 20$ that

$$dT = 7.21\,10^{-9}, \quad \Delta T = 4.35\,10^{-4}, \quad P = 114.9, \quad S = 112.3, \quad E = 0.98.$$

M = number of parareal algorithms used to get to T_{final}

What have other people used parareal for?

- Bruce Boghosian, Paul Fischer, Frederic Hecht, Yvon Maday: Navier-Stokes equations when diffusion dominant. Speed up 10-20.
- Guilaume Bal and Qi Wu (2008-2009): Symplectic parareal methods for long time orbital integrations.
    - It turns out that even when the coarse and fine solution operators are symplectic, their sums are not necessarily. So these methods require one to somehow express the parareal algorithm as a composition of sympletic operators. It is not known what the best way to do this is.

Advantages and Disadvantages

Advantages

- Allows speed up ODE solver (compared to coarse scheme with similar accuracy).
- Given a coarse and fine scheme, straightforward to implement.

Disadvantages

- Ideally the number of processors should scale N_{coarse}.
- Stability region is not simply related to that of g_{coarse}.
- Requires one to save the solutions history, or at least coordinate the corrector step appropriately.
- Requires a good understanding of the eigenvalues and stability regions on a case by case basis
  - Staff: "No multistage scheme has been found that makes the parareal algorithm stable for all [pure imaginary] eigenvalue"

Summary

- The parareal algorithm is relatively new, and is an active area of research. Applications to PDEs and ODE systems with conserved quantities are two developing areas.
- Basic theory is known: order is mk, and stability can be cumbersome or (worst) unstable.
- The standard algorithm allows a time-domain decomposition, whereby the high accurate corrections can be done in parallel.
- Numerous extension and modifications are possible.
- Speed up for ODEs appears to be a good example of usefulness: 10-1000x