Adaptive Error Control for RIDC

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Orientation

Saskatchewan

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Saskatchewan
Easy to draw, hard to spell.

Acknowledgements

- My partners in crime

C. Macdonald

B. Ong

- Support from

NSERC CRSNG / People. Discovery. Innovation.

MITACS

IBM

Outline

Deferred Correction

We are interested in solving the initial-value problem

$$\frac{d}{dt}\mathbf{y}(t) = \mathbf{f}(t, \mathbf{y}(t)), \quad t \in (t_0, t_f), \ \mathbf{y}(t) \in \mathbb{R}^m,$$
$$\mathbf{y}(t_0) = \mathbf{y}_0.$$

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Deferred Correction

Computational issues:

- $m \sim \mathcal{O}(n_{\text{grid}})$
- stiffness

Deferred Correction

Canonical algorithms:

- forward Euler (explicit)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t_n \, \mathbf{f}(t_n, \mathbf{y}_n)$$

- backward Euler (implicit)

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Deferred Correction

- serial nature
- lots of information exchange

Deferred Correction

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- lots of information exchange

How to take advantage of (massive) parallelism?

Deferred Correction

Natural strategies:

- domain decomposition
- fine-grained parallelism

Deferred Correction

Other strategies:

- specialized integrators
- extrapolation
- PARAREAL
- deferred correction

Deferred Correction

Other strategies:

- specialized integrators
- extrapolation
- PARAREAL
- deferred correction

Deferred Correction

de·fer |diˈfər|
verb (**-ferred, -fer·ring**) [trans.]
put off (an action or event) to a later time; postpone.

cor·rec·tion |kəˈrek SH ən|
noun
the action or process of correcting something;
a change that rectifies an error or inaccuracy

Deferred Correction

- first proposed by Fox (1947)
  - "difference-correction methods"
- Pereyra (1960s), Stetter (1970s), Skeel (1980s); Dutt, Greengard, and Rokhlin (2000); Minion et al. (2000s); Christlieb et al. (2010s); Emmett and Minion (2010s)
- can be applied to BVPs, DAEs, and eigenvalue problems

Deferred Correction

General idea:

1: Compute a provisional solution $\mathbf{Y}^{[0]}$.
2: **for** k=0,1,... **do**
3: Estimate the error $\mathbf{E}^{[k]}$.
4: Correct the current solution by adding error estimate:

$$\mathbf{Y}^{[k+1]} = \mathbf{Y}^{[k]} + \mathbf{E}^{[k]}.$$

5: **end for**

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Accuracy of $\mathbf{Y}^{[k+1]}$ can be $\mathcal{O}\left(\sum_{j=0}^{k} p_j\right)$!

Deferred Correction

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Pipeline!

Deferred Correction

Main classes of deferred correction methods:

- classical deferred correction
- spectral deferred correction
- integral deferred correction

All equivalent mathematically; devil in details.

Classical Deferred Correction

Consider

$$\frac{d}{dt}\mathbf{y}(t) = \mathbf{f}(t, \mathbf{y}(t)), \quad t \in (t_0, t_f),$$
$$\mathbf{y}(t_0) = \mathbf{y}_0.$$

Define the error function

$$\mathbf{e}(t, \mathbf{Y}^{[k]}(t)) = \mathbf{y}(t) - \mathbf{Y}^{[k]}(t).$$

Then

$$\frac{d}{dt}\mathbf{e}(t, \mathbf{Y}^{[k]}(t)) = \mathbf{f}(t, \mathbf{e}(t, \mathbf{Y}^{[k]}(t)) + \mathbf{Y}^{[k]}(t)) - \frac{d}{dt}\mathbf{Y}^{[k]}(t),$$
$$\mathbf{e}(t_0, \mathbf{Y}^{[k]}(t_0)) = \mathbf{0}.$$

Classical Deferred Correction

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$$\mathbf{e}(t_0, \mathbf{Y}^{[k]}(t_0)) = \mathbf{0}.$$

Spectral Deferred Correction

Rewrite the exact solution in integral form

$$\mathbf{y}(t) = \mathbf{y}_0 + \int_{t_0}^{t} \mathbf{f}(t', \mathbf{y}(t'))\, dt'.$$

Define the *residual* function

$$\mathbf{r}(t, \mathbf{Y}^{[k]}(t)) = \mathbf{y}_0 + \int_{t_0}^{t} \mathbf{f}(t', \mathbf{Y}^{[k]}(t'))\, dt' - \mathbf{Y}^{[k]}(t).$$

Then

$$\frac{d}{dt}\mathbf{e}(t, \mathbf{Y}^{[k]}(t)) = \mathbf{\Delta f_Y}(t, \mathbf{e}(t, \mathbf{Y}^{[k]}(t))) + \frac{d}{dt}\mathbf{r}(t, \mathbf{Y}^{[k]}(t)).$$

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Then

$$\frac{d}{dt}\mathbf{e}(t, \mathbf{Y}^{[k]}(t)) = \boldsymbol{\Delta}\mathbf{f}_{\mathbf{Y}}(t, \mathbf{e}(t, \mathbf{Y}^{[k]}(t))) + \frac{d}{dt}\mathbf{r}(t, \mathbf{Y}^{[k]}(t)).$$

Integral Deferred Correction

Define the *defect* function

$$\delta(t, \mathbf{Y}^{[k]}(t)) = \mathbf{f}(t, \mathbf{Y}^{[k]}(t)) - \frac{d}{dt}\mathbf{Y}^{[k]}(t).$$

Then

$$\frac{d}{dt}\left[\mathbf{e}(t, \mathbf{Y}^{[k]}(t)) - \int_{t_0}^{t} \delta(t', \mathbf{Y}^{[k]}(t'))\, dt'\right] = \mathbf{\Delta f_Y}(t, \mathbf{e}(t, \mathbf{Y}^{[k]}(t))).$$

Note:

$$\delta(t, \mathbf{Y}^{[k]}(t)) = \frac{d}{dt}\mathbf{r}(t, \mathbf{Y}^{[k]}(t)).$$

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Note:

$$\delta(t, \mathbf{Y}^{[k]}(t)) = \frac{d}{dt}\mathbf{r}(t, \mathbf{Y}^{[k]}(t)).$$

Revisionist Integral Deferred Correction

- Classically, sweep level by level.
- “Revisionist”: pipeline subsequent levels.

Error and Stepsize Control

Error control:

- Easy to imagine p-refinement.
- Consider h-refinement.
- hp-refinement: future work.

Error and Stepsize Control

Classical algorithms for error estimation based on *h*-refinement:

- Step doubling
- Embedded formulas

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Error and Stepsize Control

Step doubling:
If

$$\mathbf{e}_{n+1/2} = \mathbf{y}(t_n + \Delta t_n) - \mathbf{y}_{n+1} = C(\Delta t)^{p+1} + \mathcal{O}(\Delta t^{p+2}),$$

then

$$\mathbf{e}_{n+1} = \mathbf{y}(t_n + 2\Delta t_n) - \mathbf{y}_{n+1} = 2C(\Delta t)^{p+1} + \mathcal{O}(\Delta t^{p+2}),$$
$$\hat{\mathbf{e}}_{n+1} = \mathbf{y}(t_n + 2\Delta t_n) - \hat{\mathbf{y}}_{n+1} = \hat{C}(2\Delta t)^{p+1} + \mathcal{O}(\Delta t^{p+2}),$$

and hence

$$\mathbf{e}_{n+1} = \frac{\mathbf{y}_{n+1} - \hat{\mathbf{y}}_{n+1}}{2^p - 1} + \mathcal{O}(\Delta t^{p+2}).$$

Error and Stepsize Control

Classical algorithm for stepsize control:
Given user tolerances $\boldsymbol{\tau}_{\text{abs}}$, $\boldsymbol{\tau}_{\text{rel}}$, define

$$\boldsymbol{\tau}_{n+1} = \boldsymbol{\tau}_{\text{rel}} \max(|\mathbf{y}_n|, |\mathbf{y}_{n+1}|) + \boldsymbol{\tau}_{\text{abs}},$$

and

$$\epsilon_{n+1} = \left|\left| \frac{\mathbf{e}}{\boldsymbol{\tau}} \right|\right|_{\text{RMS}}.$$

Then

$$\Delta t_{\text{opt}} = \Delta t_n \left(\frac{1}{\epsilon_{n+1}} \right)^{\frac{1}{p+1}}$$

and

$$\Delta t_{n+1} = \alpha \min(a_{\max} \Delta t_n, \max(\Delta t_{\text{opt}}, a_{\min} \Delta t_n))$$

Error and Stepsize Control

Ideas for error and stepsize control within RIDC:

- on prediction level only
- on all levels

Test Problem 1 (Auzinger)

$$\dot{y}_1 = -y_2 + y_1(1 - y_1^2 - y_2^2),$$
$$\dot{y}_2 = y_1 + 3y_2(1 - y_1^2 - y_2^2),$$

$$y(0) = (1, 0)^T, \quad t \in [0, 10].$$

Exact solution:

$$y(t) = (\cos t, \sin t)^T.$$

Test Problem 2 (Arenstdorf)

$$\ddot{y}_1 = y_1 + 2\dot{y}_2 - \mu' \frac{y_1 + \mu}{D_1} - \mu \frac{y_1 - \mu'}{D_2},$$
$$\ddot{y}_2 = y_2 - 2\dot{y}_1 - \mu' \frac{y_2}{D_1} - \mu \frac{y_2}{D_2},$$

$$D_1 = \left((y_1 + \mu)^2 + y_2^2\right)^{3/2}, \quad D_2 = \left((y_1 - \mu')^2 + y_2^2\right)^{3/2},$$

$$\mu = 0.012277471, \quad \mu' = 1 - \mu.$$

$$y_1(0) = 0.994, \quad \dot{y}_1(0) = 0, \quad y_2(0) = 0,$$

$$\dot{y}_2(0) = -2.00158510637908252240537862224.$$

Solution has period $t_{end} = 17.0652165601579625588917206249.$

Order Verification

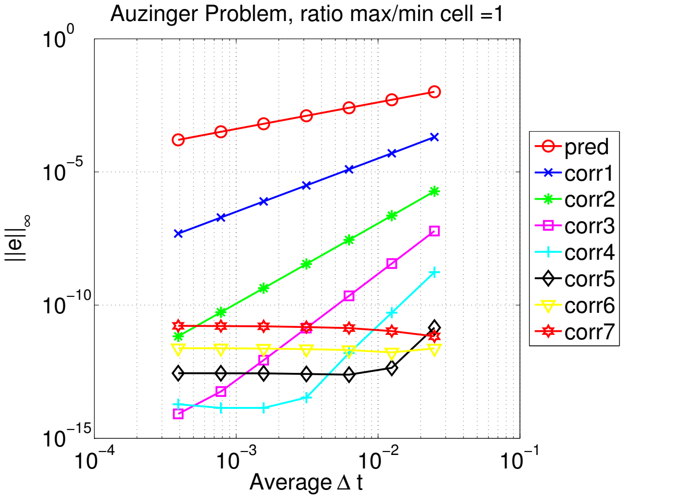
Randomize the step size according to

$$t_{n+1}^{[k]} = t_n^{[k]} + \Delta t_n^{[k]}, \quad k = 0, 1, \ldots, K, \quad n = 0, 1, \ldots,$$

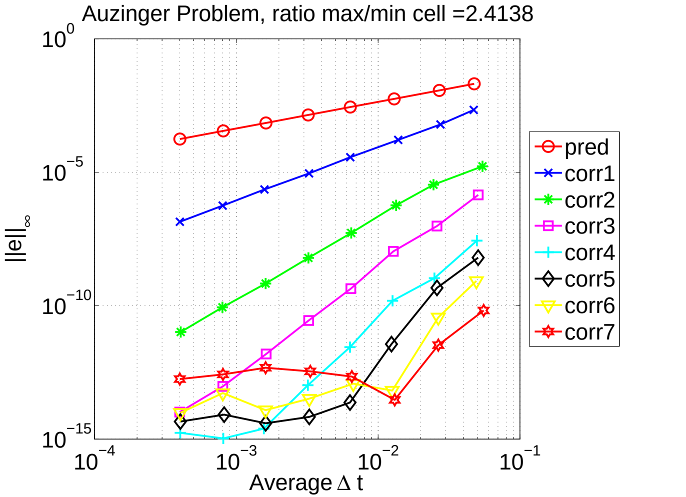
where $\Delta t_n^{[k]}$ is randomly selected from

$$\left[\frac{1}{\omega}\Delta t_{n-1}^{[k]}, \omega \Delta t_{n-1}^{[k]}\right], \quad \omega \geq 1.$$

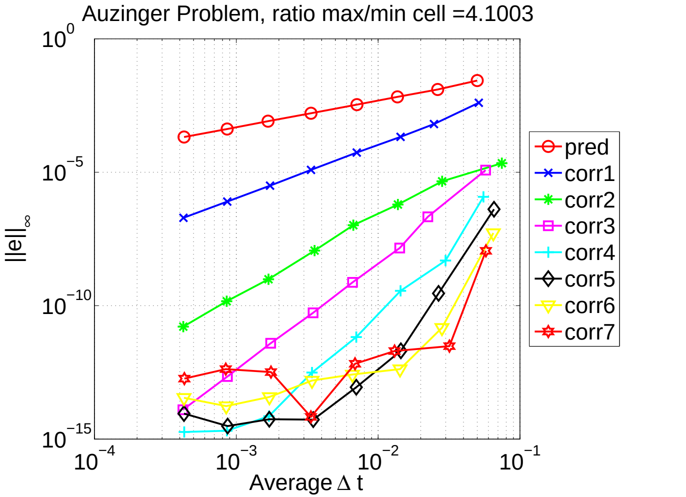
Results


Auzinger Problem, ratio max/min cell =1
10^{0}
10^{-5}
10^{-10}
10^{-15}
$||e||_\infty$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Average Δ t
pred
corr1
corr2
corr3
corr4
corr5
corr6
corr7

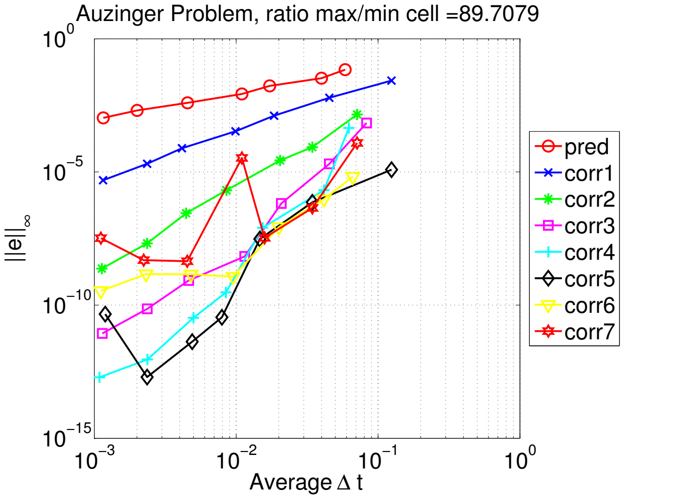
Results


Auzinger Problem, ratio max/min cell =2.4138
10^{0}
10^{-5}
10^{-10}
10^{-15}
$\|e\|_\infty$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Average Δ t
pred
corr1
corr2
corr3
corr4
corr5
corr6
corr7

Results


Auzinger Problem, ratio max/min cell =4.1003
10^{0}
10^{-5}
10^{-10}
10^{-15}
$||e||_\infty$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Average Δ t
pred
corr1
corr2
corr3
corr4
corr5
corr6
corr7

Results

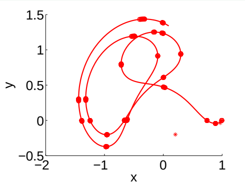

Auzinger Problem, ratio max/min cell =89.7079
10^0
10^{-5}
10^{-10}
10^{-15}
$||e||_\infty$
10^{-3}
10^{-2}
10^{-1}
10^0
Average Δ t
pred
corr1
corr2
corr3
corr4
corr5
corr6
corr7

Error and Stepsize Control on Prediction Level Only

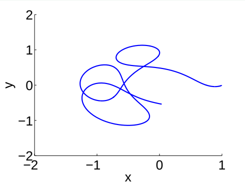
First idea:

- Perform standard error and stepsize control on prediction level.
- Use same stepsizes on remaining levels.

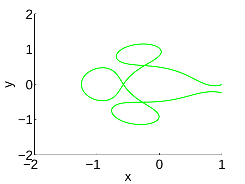
Results (Orbit Problem)



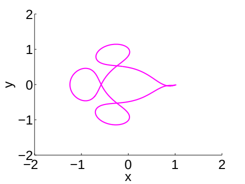
(a) Level 0



(b) Level 1



(c) Level 2



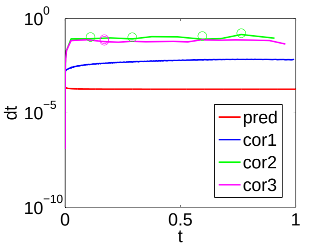
(d) Level 3

Error and Stepsize Control on All Levels

Better idea:

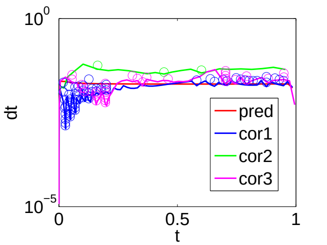
- Perform standard error and stepsize control on all levels.
- Tolerance settings:
  - Same at every level.
  - Loose at first, gradually tighten.
- How to sensibly set tolerances: future work.

Results (Auzinger Problem)



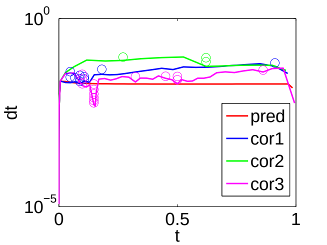
ℓ	rtol	atol	error	naccept	nreject
0	10^{-8}	10^{-10}	2.028e-05	5480	0
1	10^{-8}	10^{-10}	8.824e-07	197	0
2	10^{-8}	10^{-10}	1.917e-08	19	4
3	10^{-8}	10^{-10}	6.386e-07	25	2

Results (Auzinger Problem)



p	rtol	atol	error	naccept	nreject
0	1e-04	1e-06	2.031e-03	59	0
1	1e-06	1e-08	7.002e-05	81	61
2	1e-08	1e-10	1.412e-07	30	3
3	1e-10	1e-12	9.847e-08	60	33

Results (Auzinger Problem)



p	rtol	atol	error	naccept	nreject
0	1e-04	1e-06	2.031e-03	59	0
1	1e-05	1e-07	1.853e-04	31	10
2	1e-07	1e-09	1.505e-06	21	3
3	1e-09	1e-11	9.473e-07	44	14

Conclusions

- Deferred correction is a well-studied idea
- RIDC is a framework that allows for parallelization
- Error and stepsize control can be implemented in RIDC