Defect correction as a family of iterative techniques for ODEs

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Contents

Problem class: ODE systems (IVP, BVP)

- ODE system:

$$y'(t) = f(t, y(t)), \qquad t \in [t_{start}, t_{end}]$$

  - with initial or boundary conditions
  - exact solution $y^*(t)$

- In this talk:

  'Classical' smoothness assumptions
  (non-stiff, non-singular)

Test problem (autonomous, non-stiff)

IVP:

$$\begin{aligned} y'(t) &= f(t, y(t)), \\ y(0) &= y_{start} \end{aligned}$$

with

$$f(t, y) = \begin{pmatrix} -y_2 + y_1(1 - y_1^2 - y_2^2) \\ y_1 + 3y_2(1 - y_1^2 - y_2^2) \end{pmatrix}$$

Solution: $y^*(t) = (\cos t, \sin t)^T$

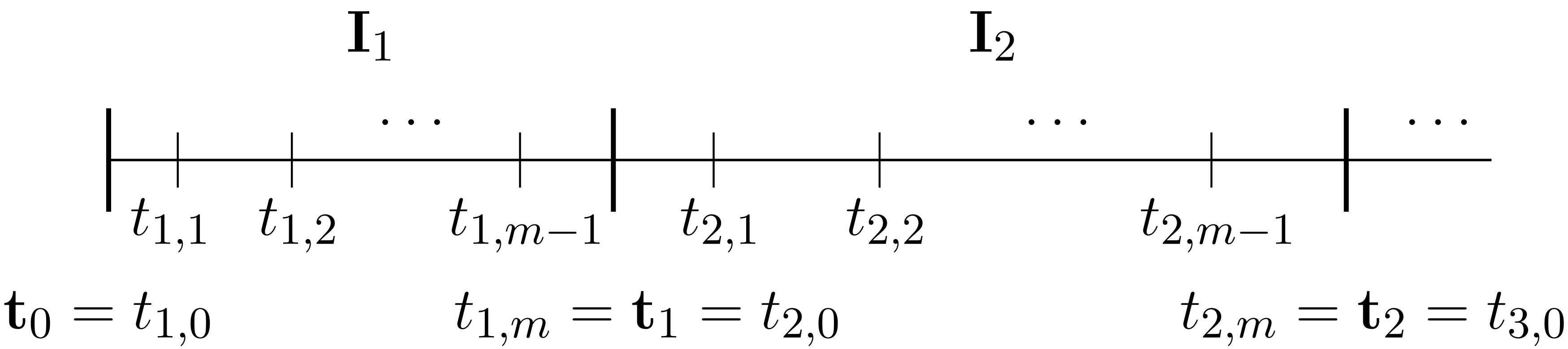
Classical IDeC = Iterated Defect Correction

- $\eta_h^{[0]}$ . . . basic approximation (e.g. by Euler scheme)
- Iteration $[\nu] \mapsto [\nu+1]$:
  - Interpolate: $\eta_h^{[\nu]} \mapsto p^{[\nu]}(t)$ (degree m)
  - Compute defect of $p^{[\nu]}(t)$ w.r.t. given ODE:

$$d^{[\nu]}(t) := \frac{d}{dt} p^{[\nu]}(t) - f(t, p^{[\nu]}(t)) \quad \text{(small)}$$

  - Solve modified ODE: $y' = f(t,y) + d^{[\nu]}(t)$
    (exact solution $p^{[\nu]}(t)!$) by basic scheme $\rightarrow \hat{\eta}_h^{[\nu]}$
  - New approximation: $\eta_h^{[\nu+1]} := \eta_h^{[\nu]} - \underbrace{(\hat{\eta}_h^{[\nu]} - \eta_h^{[0]})}_{\text{estimate for } \eta_h^{[\nu]} - y^*}$

Grid, interpolation intervals



- $t_{j,\ell}$ . . . grid points (basic scheme, interpolation), $h_{j,\ell} := t_{j,\ell} - t_{j,\ell-1}$
- $\mathbf{I}_j = [\mathbf{t}_{j-1}, \mathbf{t}_j]$ . . . interpolation intervals, $\mathbf{h}_j := \mathbf{t}_j - \mathbf{t}_{j-1}$
- Tables to follow: degree $m = 4$

IDeC on equidistant grid: O.K.

Basic scheme: Backward Euler (BEUL)

TARGET = iteration limit ($\nu \to \infty$ on fixed grid)

Global error (at $t = 3$), observed order:

$\mathbf{h}$	BEUL	IDeC 1	IDeC 2	IDeC 3	IDeC 4	TARGET
0.200	9.00E-03	5.37E-04	6.74E-05	6.89E-06	1.06E-06	1.45E-06
0.100	4.50E-03	1.42E-04	9.37E-06	4.75E-07	7.92E-08	9.11E-08
0.050	2.25E-03	3.64E-05	1.24E-06	3.10E-08	5.36E-09	5.70E-09
0.025	1.13E-03	9.22E-06	1.59E-07	1.98E-09	3.34E-10	3.56E-10
0.200						
	1.00	1.92	2.85	3.86	3.74	4.00
0.100						
	1.00	1.96	2.92	3.94	3.89	4.00
0.050						
	1.00	1.98	2.96	3.97	4.00	4.00
0.025						

$\mathbf{h} \downarrow 0$: order limited by $\mathcal{O}(\mathbf{h}^m)$ ($m \ldots$ polynom. degree)

IDeC on nonequidistant grid: iteration stalls

Basic scheme: Backward Euler (BEUL)

Global error (at $t = 3$), observed order:

h	BEUL	IDeC 1	IDeC 2	IDeC 3	IDeC 4	TARGET
0.200	1.19E-02	1.26E-03	4.20E-03	3.31E-03	3.71E-04	1.07E-06
0.100	6.07E-03	3.42E-04	1.36E-03	1.55E-03	2.04E-04	6.68E-08
0.050	3.06E-03	1.03E-04	4.81E-04	7.64E-04	1.04E-04	4.17E-09
0.025	1.54E-03	3.66E-05	1.94E-04	3.83E-04	5.88E-05	2.61E-10
0.200						
	0.98	1.88	1.63	1.10	0.87	4.00
0.100						
	0.99	1.73	1.50	1.02	0.96	4.00
0.050						
	0.99	1.49	1.31	1.00	0.83	4.00
0.025						

(grid points $t_{j,\ell}$ chosen at random)

Collocation = target scheme of IDeC iteration

- Defect $d(t_{j,\ell}) = p'(t_{j,\ell}) - f(t_{j,\ell}, p(t_{j,\ell})) = 0$ if evaluated for collocation solution $p(t) = p^{[coll]}(t)$
- $\Rightarrow$ $p^{[coll]}(t) =$ fixed point of IDeC iteration
- I.e.: Collocation is target scheme of IDeC
- Collocation equations:

$$\frac{d}{dt} p^{[coll]}(t_{j,\ell}) = f(t_{j,\ell}, p^{[coll]}(t_{j,\ell}))$$

- … equivalent to Runge-Kutta equations:

$$\frac{p^{[coll]}_{j,\ell} - \mathbf{p}^{[coll]}_{j-1}}{\mathbf{h}_j} = \sum_{\mu=1}^{m} a_{\ell,\mu}\, f(t_{j,\mu}, p^{[coll]}_{j,\mu})$$

Collocation and (modified) Runge-Kutta

- . . . equivalent to modified Runge-Kutta equations, i.e. Runge-Kutta rewritten as

$$\frac{p_{j,\ell}^{[coll]} - p_{j,\ell-1}^{[coll]}}{h_{j,\ell}} = \sum_{\mu=1}^{m} \alpha_{\ell,\mu} \underbrace{f(t_{j,\mu}, p_{j,\mu}^{[coll]}}_{= \frac{d}{dt} p_j^{[coll]}(t_{j,\mu})})$$

- $\{\alpha_{\ell,\mu}\}$ . . . set of local quadrature coefficients
- Important: Form of the left hand side above is the same as in basic scheme (BEUL):

$$\frac{\eta_{j,\ell} - \eta_{j,\ell-1}}{h_{j,\ell}} = f(t_{j,\ell}, \eta_{j,\ell})$$

IQDeC: IDeC with defect Quadrature

- Basic scheme: BEUL, iteration as before, but:
- use (modified) Q-defect $\bar{d}_{j,\ell}^{[\nu]}$ ...
  = residual w.r.t. modified Runge-Kutta equations
- ... equivalent to defect Quadrature =
  = local weighting with quadrature coefficients $\alpha_{\ell,\mu}$:

$$\bar{d}_{j,\ell}^{[\nu]} = \frac{\eta_{j,\ell}^{[\nu]} - \eta_{j,\ell-1}^{[\nu]}}{h_{j,\ell}} - \sum_{\mu=1}^{m} \alpha_{\ell,\mu}\, f(t_{j,\mu}, \eta_{j,\mu}^{[\nu]}) =$$

$$= \sum_{\mu=1}^{m} \alpha_{\ell,\mu}\, \underbrace{d^{[\nu]}(t_{j,\mu})}_{\uparrow}$$

classical (pointwise) defect

- all other algorithmic details as before

IQDeC on nonequidistant grid: O.K.

Basic scheme: Backward Euler (BEUL)

Global error (at $t = 3$), observed order:

h	BEUL	IQDeC 1	IQDeC 2	IQDeC 3	IQDeC 4	TARGET
0.200	1.19E-02	2.44E-03	7.31E-05	7.98E-06	1.10E-06	1.07E-06
0.100	6.07E-03	5.99E-04	8.10E-06	4.94E-07	6.66E-08	6.68E-08
0.050	3.06E-03	1.48E-04	9.65E-07	3.07E-08	4.15E-09	4.17E-09
0.025	1.54E-03	3.69E-05	1.18E-07	1.91E-09	2.60E-10	2.61E-10
0.200						
	0.98	2.03	3.17	4.01	4.05	4.00
0.100						
	0.99	2.01	3.07	4.01	4.01	4.00
0.050						
	0.99	2.01	3.03	4.01	4.00	4.00
0.025						


Das polytechnische Institut in Wien, erbaut 1816.

I$\color{blue}{Q}$DeC - convergence: Sketch of proof (shorthand notation)

- Let $\partial_h \, \eta_h \; = $ difference quotient $\frac{\eta_{j,\ell} - \eta_{j,\ell-1}}{h_{j,\ell}}$
- Basic scheme = BEUL on *arbitrary* grid:

$$\partial_h \, \eta_h^{[0]} \; = \; f(\eta_h^{[0]})$$

- Target scheme (= collocation =)
  = modified Runge-Kutta: $\partial_h \, p^{[coll]} \; = \; Q\, f(p^{[coll]})$
- Q-defect of $\eta_h^{[0]}$:

$$\bar{d}_h^{[0]} \; := \; \partial_h \, \eta_h^{[0]} - Q\, f(\eta_h^{[0]}) \; = \; (f - Q\, f)(\eta_h^{[0]})$$

- Neighboring BEUL: $\partial_h \, \hat{\eta}_h^{[0]} \; = \; f(\hat{\eta}_h^{[0]}) + \bar{d}_h^{[0]}$
- New approximation: $\eta_h^{[1]} \; := \; \eta_h^{[0]} - (\hat{\eta}_h^{[0]} - \eta_h^{[0]})$

IQDeC - convergence: Sketch of proof (2)

- Error w.r.t. target $p^{[coll]}$:

$$\varepsilon_h^{[0]} = \mathcal{O}(\mathbf{h}), \;\; \partial_h\, \varepsilon_h^{[0]} = \mathcal{O}(\mathbf{h}); \qquad \underbrace{\varepsilon_h^{[1]}}_{new} = \underbrace{\varepsilon_h^{[0]}}_{old} - \underbrace{\hat{\varepsilon}_h^{[0]}}_{old},$$

- Difference equation for $\varepsilon_h^{[0]} = \eta_h^{[0]} - p^{[coll]}$:

$$\begin{aligned} \partial_h\, \varepsilon_h^{[0]} &= f(\eta_h^{[0]}) - f(p^{[coll]}) + (f - Q f)(p^{[coll]}) \\ &= Df \cdot \varepsilon_h^{[0]} + (f - Q f)(p^{[coll]}) \end{aligned}$$

- Difference equation for $\hat{\varepsilon}_h^{[0]} = \hat{\eta}_h^{[0]} - \eta_h^{[0]}$:

$$\begin{aligned} \partial_h\, \hat{\varepsilon}_h^{[0]} &= f(\hat{\eta}_h^{[0]}) - f(\eta_h^{[0]}) + (f - Q f)(\eta_h^{[0]}) \\ &= \hat{D}f \cdot \hat{\varepsilon}_h^{[0]} + (f - Q f)(\eta_h^{[0]}) \end{aligned}$$

IQDeC - convergence: Sketch of proof (3)

- $\Rightarrow$ Difference equation for $\varepsilon_h^{[1]} = \eta_h^{[1]} - p^{[coll]}$:

$$\begin{aligned} \partial_h \, \varepsilon_h^{[1]} &= \partial_h \, \varepsilon_h^{[0]} - \partial_h \, \hat{\varepsilon}_h^{[0]} \\ &= Df \cdot \varepsilon_h^{[1]} + (f - Q\,f)(\varepsilon_h^{[0]}) + \mathcal{O}(\mathbf{h}^2) \end{aligned}$$

- Estimate of inhomogeneous term:

$$\| \, (f - Q\,f)(\varepsilon_h^{[0]}) \, \| \le \mathcal{C} \cdot \mathbf{h} \cdot \underbrace{\| \, \partial_h \, \varepsilon_h^{[0]} \, \|}_{\mathcal{O}(\mathbf{h})} + \mathcal{O}(\mathbf{h}^2) \; = \; \mathcal{O}(\mathbf{h}^2)$$

- Stability of BEUL $\Rightarrow$ estimate for $\varepsilon_h^{[1]}$ and $\partial_h \, \varepsilon_h^{[1]}$:

$$\varepsilon_h^{[1]} = \mathcal{O}(\mathbf{h}^2), \quad \partial_h \, \varepsilon_h^{[1]} = \mathcal{O}(\mathbf{h}^2)$$

- Induction $\Rightarrow$

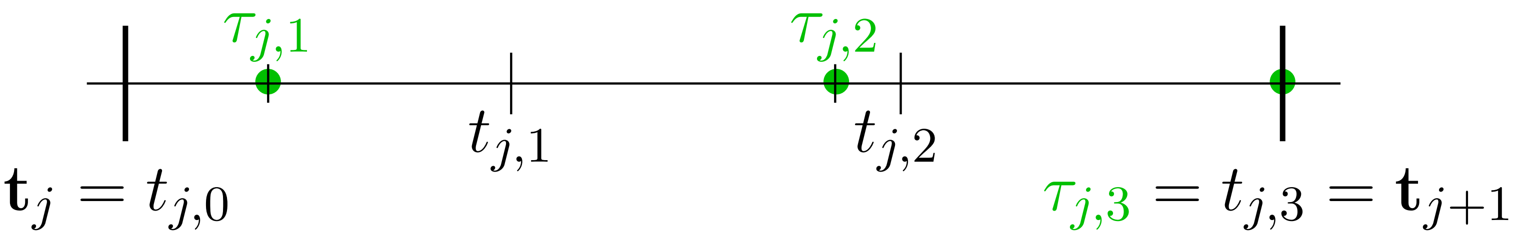
$$\varepsilon_h^{[\nu]} = \mathcal{O}(\mathbf{h}^{\nu+1}), \; \partial_h \, \varepsilon_h^{[\nu]} = \mathcal{O}(\mathbf{h}^{\nu+1}), \quad \nu = 0, 1, 2, \ldots$$

✓

IPDeC: IDeC with defect interPolation

- Wanted: Algorithmic combination of equidistant nonequidistant grids, such that
  - basic scheme works with constant step size h (most desirable for implicit schemes, IVP case)
  - target scheme defined w.r.t. nonequidistant grid (superconvergent collocation)
- Realization:
  - basic scheme (e.g. BEUL) as before, on piecewise equidistant grid $\{t_{j,\ell}\}$
  - Interpolate defect at nonequistant nodes $\{\tau_{j,k}\}$
  - use interpolated defect $\tilde{d}(t)$ instead of $d(t)$
  - $\Rightarrow$ target scheme = collocation at the $\{\tau_{j,k}\}$!

Example: equidistant / Radau nodes



- $t_{j,\ell}$ . . . grid points (for basic scheme)
- $\tau_{j,k}$ . . . nodes for defect interpolation
- Interpolated defect $\tilde{d}(t) \equiv 0$ for Radau collocation
- $\Rightarrow$ Radau is target scheme
- Convergence: ✓ Proof: ✓

IPDeC using ‘Radau’ defect

Basic scheme: Backward Euler (BEUL)

Target scheme: Radau IIa collocation, degree $m = 3$

Global error (at $t = 3$) ... superconvergence $2m - 1$:

$\mathbf{h}$	BEUL	IPDeC 1	IPDeC 2	IPDeC 3	IPDeC 4	RADAU
0.200	1.20E-02	9.13E-04	1.62E-04	1.50E-05	1.84E-06	1.22E-07
0.100	6.00E-03	2.47E-04	2.25E-05	1.14E-06	6.79E-08	3.86E-09
0.050	3.00E-03	6.41E-05	2.96E-06	7.82E-08	2.30E-09	1.21E-10
0.025	1.50E-03	1.63E-05	3.79E-07	5.10E-09	7.47E-11	3.78E-12
0.200						
	1.00	1.89	2.85	3.71	4.76	4.99
0.100						
	1.00	1.95	2.93	3.87	4.88	5.00
0.050						
	1.00	1.97	2.96	3.94	4.94	5.00
0.025						

IPDeC: symmetric version using ‘Gauss’ defect

Basic scheme: Implicit Trapezoidal Rule (ITR)

Target scheme: Gauss collocation, degree $m = 3$

Global error (at $t = 3$) ... superconvergence $2m$:

h	ITR	IPDeC 1	IPDeC 2	IPDeC 3	GAUSS
0.200	1.11E-03	1.29E-06	2.07E-08	1.75E-09	1.79E-09
0.100	2.78E-04	8.06E-08	3.26E-10	2.87E-11	2.88E-11
0.050	6.94E-05	5.04E-09	5.10E-12	4.53E-13	4.54E-13
0.025	1.74E-05	3.15E-10	7.99E-14	5.59E-15	6.57E-15
0.200					
	2.00	4.00	5.99	5.93	5.96
0.100					
	2.00	4.00	6.00	5.99	5.99
0.050					
	2.00	4.00	6.00	6.34	6.11
0.025					

Conclusion

- General template for computing defects: by preconditioning (weighting), i.e.

$$d_{j,\ell}^{modified} = \sum_{\mu=1}^{m} \omega_{\ell,\mu} \underbrace{d^{[\nu]}(t_{j,\mu})}_{\uparrow}$$

classical (pointwise) defect

- In contrast to classical IDeC:
  - Full grid flexibility
  - Superconvergence

- Stiff problems $\Rightarrow$ talk by H. Hofstätter
- Related material $\Rightarrow$ talks by O. Koch, E. Weinmüller