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High Order Lobatto-Obrechkoff Integration Formulae for the Solution of Two Point Boundary Value Problems

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Statement of the Problem

We wish to solve nonlinear two point boundary value problems of the form:

$$y'' = \begin{cases} f(x,\ y) \\ f(x,\ y,\ y') \end{cases},\quad x \in [a,\ b], \tag{1}$$

subject to the nonlinear non-separated boundary conditions:

$$g(y(a),\ y(b)) = 0. \tag{2}$$

Solving BVPs Numerically

Boundary value problem solvers can be divided into two main classes:

- *IVP Methods*: The problem is reformulated in terms of an Initial Value Problem. Shooting methods being one example, where the initial conditions are varied until both boundary conditions are satisfied.
- *Finite difference methods*, of which there are the following prominent subclasses:
  - *Collocation methods*: one seeks a continuous solution to the BVP. These are typically expressed in terms of a monomial basis, but other examples include Chebyshev functions and B-Splines.
  - *Mesh point methods*: a solution is sought at a finite set of mesh points.

Mesh Point Methods

We partition our domain into M points:

$$\left[x_1,\ x_2,\ x_3,\ \ldots,\ x_{M-1},\ x_M\right],\ x_i < x_{i+1}\ \forall i,\ x_1 = a,\ x_M = b, \tag{3}$$

and we wish to find the following mesh points:

$$\left[y_1,\ y_2,\ \ldots,\ y_{M-1},\ y_M\right]. \tag{4}$$

This is done by solving the following one-step finite difference scheme for the $M - 1$ mesh point intervals $[y_n,\ y_{n+1}]$:

$$\frac{y_{n+1} - y_n}{x_{n+1} - x_n} = F\left(x_n,\ x_{n+1},\ y_n,\ y_{n+1}\right). \tag{5}$$

We refer to F as our *finite difference scheme*.

Finite difference schemes ($y' = f(x,y)$)

Two famous examples are:

- *Trapezium rule*:

$$F\left(x_n,\ x_{n+1},\ y_n,\ y_{n+1}\right) = \frac{f\left(x_n,\ y_n\right) + f\left(x_{n+1},\ y_{n+1}\right)}{2}. \tag{6}$$

- *Keller's box scheme*:

$$F\left(x_n,\ x_{n+1},\ y_n,\ y_{n+1}\right) = f\left(x_{n+\frac{1}{2}},\ y_{n+\frac{1}{2}}\right), \tag{7}$$

where,

$$x_{n+\frac{1}{2}} = \frac{x_n + x_{n+1}}{2}, \qquad y_{n+\frac{1}{2}} = \frac{y_n + y_{n+1}}{2}. \tag{8}$$

Finite difference schemes ($y' = f(x,y)$) (2)

If we compute the local truncation error of the trapezium and midpoint schemes,

$$\epsilon_{\text{lte}} = \frac{y_{n+1} - y_n}{h_n} - F\left(x_n,\ \ x_{n+1},\ \ y_n,\ \ y_{n+1}\right), \tag{9}$$

we find that $\epsilon_{\text{lte}} \approx O(h_n^2)$ for both schemes. For the trapezium rule we have:

$$\frac{y_{n+1} - y_n}{h_n} - \frac{f\left(x_n,\ \ y_n\right) + f\left(x_{n+1},\ \ y_{n+1}\right)}{2} = -\frac{h_n^2}{12}\frac{\mathrm{d}^3 y}{\mathrm{d}x^3} + O(h_n^3). \tag{10}$$

These schemes are of order 2.

Two Schemes of Order 4

A Gauss Scheme –

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{11}$$

A Lobatto IIIA Scheme (a.k.a. Clippinger-Dimsdale):

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

$$\begin{aligned} y_{n+\frac{1}{2}} &= \tfrac{1}{2}(y_n + y_{n+1}) + \tfrac{h_n}{8}(y'_{n+1} - y'_n) \\ F &= \tfrac{1}{6}\Big(f\left(x_n,\ y_n\right) + 4f\left(x_{n+\frac{1}{2}},\ y_{n+\frac{1}{2}}\right) \\ &\quad + f\left(x_{n+1},\ y_{n+1}\right)\Big) \end{aligned} \tag{12}$$

Two Schemes of Order 4 (2)

From the previous slide, it is apparent that:

- For the Gauss scheme: given a y_n and y_{n+1}, one then has to perform a numerical solve in order to compute $y_{n+\frac{1}{2}\pm\frac{\sqrt{3}}{6}}$.
- An explicit formulation can be found for the point $y_{n+\frac{1}{2}}$, when using the Lobatto IIIA scheme.

We denote schemes that have explicit expressions for the internal points as being Mono Implicit Runge-Kutta (MIRK) schemes. The order of the scheme is usually added as a suffix.

MIRK schemes

MIRK schemes posses the following strengths/weaknesses:

- As the internal points are computed explicitly, MIRK schemes are cheap to compute. Hence are *very* quick to solve for.
- MIRK schemes do not have a uniformly high stage order $\left(y_{n+\omega} - y\left(x_{n+\omega}\right)\right)$. Rendering them both:
    - Difficult to derive (especially for higher orders).
    - Hard to pass high order interpolants through.
- MIRK schemes are not well suited for solving very stiff problems, e.g. singular perturbation problems:

$$\epsilon y'' = f(x,\ y) \qquad |\epsilon| << 1. \tag{13}$$

MIRK Schemes (2)

MIRK schemes can be broken down into two constituent components:

- A quadrature formula: Of at least the same order as that desired for the integration scheme. MIRK 8 (Cash-Singhal 1982) and MIRK 10 (Capper-Moore 2005) have quadrature formulae of greater order than the scheme.
- Internal points: Most of which are of lower order than the scheme.

When deriving MIRK schemes, one usually chooses a quadrature formula, computes the internal points from:

$$\left\{ y_n, \;\; y_{n+1}, \;\; y_n', \;\; y_{n+1}' \right\}, \tag{14}$$

and then cancels out the appropriate error terms.

Bootstrapping

- From $\{y_n,\ \ y_{n+1},\ \ y'_n,\ \ y'_{n+1}\}$ we can derive at most $O(h_n^4)$ accurate points, using a Hermite-Birkhoff interpolant.
- Let's compute a point $y^{(4)}_{n+\frac{1}{2}-\alpha_1}$. $\alpha_1 \in \left[0, \frac{1}{2}\right)$.
- From $\left\{y_n,\ \ y_{n+1},\ \ y'_n,\ \ y'_{n+1},\ \ y'^{(4)}_{n+\frac{1}{2}-\alpha_1}\right\}$ we can derive at most $O(h_n^5)$ accurate points.

We carry out *bootstrapping* to find: $y^{(4)}_{n+\frac{1}{2}\pm\alpha_1}$, $y^{(5)}_{n+\frac{1}{2}\pm\alpha_2}$, . . . , but one needs to be careful when considering the errors:

$$f\left(x_{n+\frac{1}{2}-\alpha_1},\ y'^{(4)}_{n+\frac{1}{2}-\alpha_1}\right) - y\left(x_{n+\frac{1}{2}-\alpha_1}\right) = -\frac{h_n^4}{384}(4\alpha_1^2-1)^2\frac{\partial f}{\partial y}\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}$$
$$+\frac{h_n^5}{3840}(4\alpha_1^2-1)^2\left((2\alpha_1-5)\frac{\partial f}{\partial y}\frac{\mathrm{d}^5 y}{\mathrm{d}x^5}+10\left(\alpha_1-\frac{1}{2}\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y}\right)\frac{\mathrm{d}^4 y}{\mathrm{d}x^4}\right)+O(h_n^6)$$

Extension to y'' problems

If we double the size of the system, we can divide meshpoints up into two distinct components:

$$z_n = \begin{pmatrix} y_n \\ y'_n \end{pmatrix}, \tag{15}$$

the system is solved for z_n and z_{n+1}, effectively giving us:

$$\left\{ y_n,\ \ y_{n+1},\ \ y'_n,\ \ y'_{n+1},\ \ y''_n,\ \ y''_{n+1} \right\}. \tag{16}$$

Thus we are able to compute order 6 points without the need for bootstrapping.

Hermite-Birkhoff Interpolants

We start with the following interpolant:

$$y_{n+\omega} = A(\omega)y_{n+1} + (1 - A(\omega))y_n + h_n(B(\omega)y'_{n+1} - B(1-\omega)y'_n) \\ + h_n^2(C(\omega)y''_{n+1} + C(1-\omega)y''_n), \quad (17)$$

where,

$$\begin{aligned} A(\omega) &= \omega^3(6\omega^2 - 15\omega + 10) \\ B(\omega) &= \omega^3(3\omega - 4)(1-\omega) \\ C(\omega) &= \tfrac{1}{2}\omega^3(1-\omega)^2 \end{aligned} \quad , \quad (18)$$

and,

$$y'_{n+\omega} - y'(x_n + \omega h_n) = -\frac{1}{120}(\omega - 1)^2\left(\omega - \frac{1}{2}\right)\omega^2 \frac{\mathrm{d}^6 y}{\mathrm{d}x^6} h_n^5 + \text{h.o.t.} \quad (19)$$

LOB 6

We use a Lobatto quadrature formulae:

$$y'_{n+1} = y'_n + \frac{h_n}{12}\left((y''_{n+1} + y''_n) + 5\left(y''_{n+\frac{1}{2}+\frac{\sqrt{5}}{10}} + y''_{n+\frac{1}{2}-\frac{\sqrt{5}}{10}} \right)\right). \qquad (20)$$

A companion Obrechkoff type formula using the same values of y'' may also be derived:

$$y_{n+1} = y_n + \frac{h_n}{2}(y'_{n+1} + y'_n) - \frac{h_n^2}{24}\left((y''_{n+1} - y''_n) + \sqrt{5}\left(y''_{n+\frac{1}{2}+\frac{\sqrt{5}}{10}} - y''_{n+\frac{1}{2}-\frac{\sqrt{5}}{10}} \right)\right). \qquad (21)$$

To highlight their difference to MIRK schemes, we denote these schemes as Lobatto-Obrechkoff (LOB) schemes.

LOB 6 (2)

The internal points are computed as follows:

$$y^{(6)}_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}} = \frac{125\pm 41\sqrt{5}}{250} y_{n+1} + \frac{125\mp 41\sqrt{5}}{250} y_n - h_n \left(\frac{15\pm 4\sqrt{5}}{125} y'_{n+1} - \frac{15\mp 4\sqrt{5}}{125} y'_n \right) + h_n^2 \left(\frac{5\pm\sqrt{5}}{500} y''_{n+1} + \frac{5\mp\sqrt{5}}{500} y''_n \right), \tag{22}$$

where,

$$y'^{(5)}_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}} = \frac{6(y_{n+1}-y_n)}{5\,h_n} - \frac{5\mp 7\sqrt{5}}{50} y'_{n+1} - \frac{5\pm 7\sqrt{5}}{50} y'_n \mp \frac{h_n\sqrt{5}}{50} \left(y''_{n+1} + y''_n \right). \tag{23}$$

The derivatives are then computed:

$$y''_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}} = \begin{cases} f\left(x_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}},\ y^{(6)}_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}} \right) & \text{for } y'' = f(x,\ y) \text{ problems.} \\ f\left(x_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}},\ y^{(6)}_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}},\ y'^{(5)}_{n+\frac{1}{2}\pm\frac{\sqrt{5}}{10}} \right) & \text{for } y'' = f(x,\ y,\ y') \text{ problems.} \end{cases} \tag{24}$$

$f(x,\ y,\ y')$ and $f(x,\ y)$ problems

- $y'' = f(x,\ y)$ problems do not require one to compute intermediate $y'_{n+\omega}$ values. Their truncation errors are also easier to compute:

$$y'_{n+1} - y'_n - \frac{h_n}{12}\left(\left(y''_{n+1} + y''_n\right) + 5\left(y''_{n+\frac{1}{2}+\frac{\sqrt{5}}{10}} + y''_{n+\frac{1}{2}-\frac{\sqrt{5}}{10}} \right)\right) = \frac{h_n^7}{504000}\left[2\frac{\mathrm{d}^7 y}{\mathrm{d}x^7} - 7\frac{\partial f}{\partial y'}\frac{\mathrm{d}^6 y}{\mathrm{d}x^6}\right] + O(h_n^8), \tag{25}$$

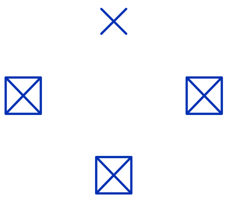
$$y_{n+1} - y_n - \frac{h_n}{2}\left(y'_{n+1} + y'_n\right) + \frac{h_n^2}{24}\left(\left(y''_{n+1} - y''_n\right) + \sqrt{5}\left(y''_{n+\frac{1}{2}+\frac{\sqrt{5}}{10}} - y''_{n+\frac{1}{2}-\frac{\sqrt{5}}{10}} \right)\right) = \frac{h_n^7}{1512000}\left[\left(21\frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial f}{\partial y'} - 14\frac{\partial f}{\partial y}\right)\frac{\mathrm{d}^6 y}{\mathrm{d}x^6} + \frac{\partial f}{\partial y'}\frac{\mathrm{d}^7 y}{\mathrm{d}x^7} - \frac{\mathrm{d}^8 y}{\mathrm{d}x^8}\right] + O(h_n^8). \tag{26}$$

Bootstrapping for higher order methods

LOB 6

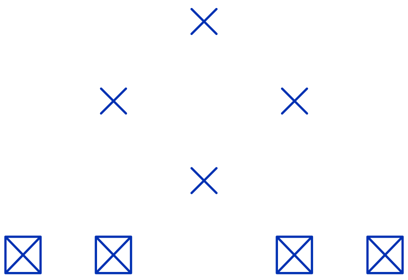
α_1	$O(h_n^{6,5})$

LOB 8



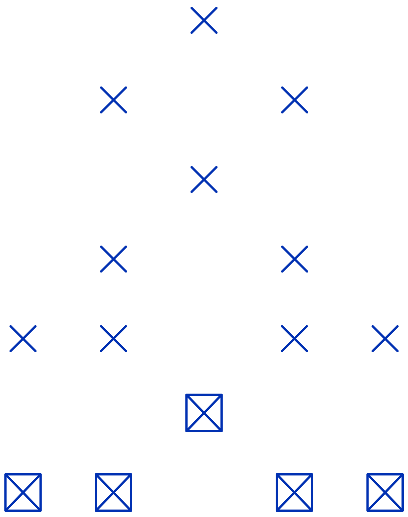
	$O(h_n^{6,6})$
α_1	$O(h_n^{7,6})$
	$O(h_n^{9,7})$

LOB 10



	$O(h_n^{6,6})$
α_1	$O(h_n^{7,7})$
	$O(h_n^{8,8})$
α_2, α_3	$O(h_n^{9,8})$

LOB 12



	$O(h_n^{6,6})$
α_1	$O(h_n^{7,7})$
	$O(h_n^{8,8})$
α_2	$O(h_n^{9,8})$
α_3, α_4	$O(h_n^{9,9})$
	$O(h_n^{12,10})$
α_5, α_6	$O(h_n^{11,10})$

Number of Internal Function Evaluations

The numbers of internal function evaluations required for each scheme are:

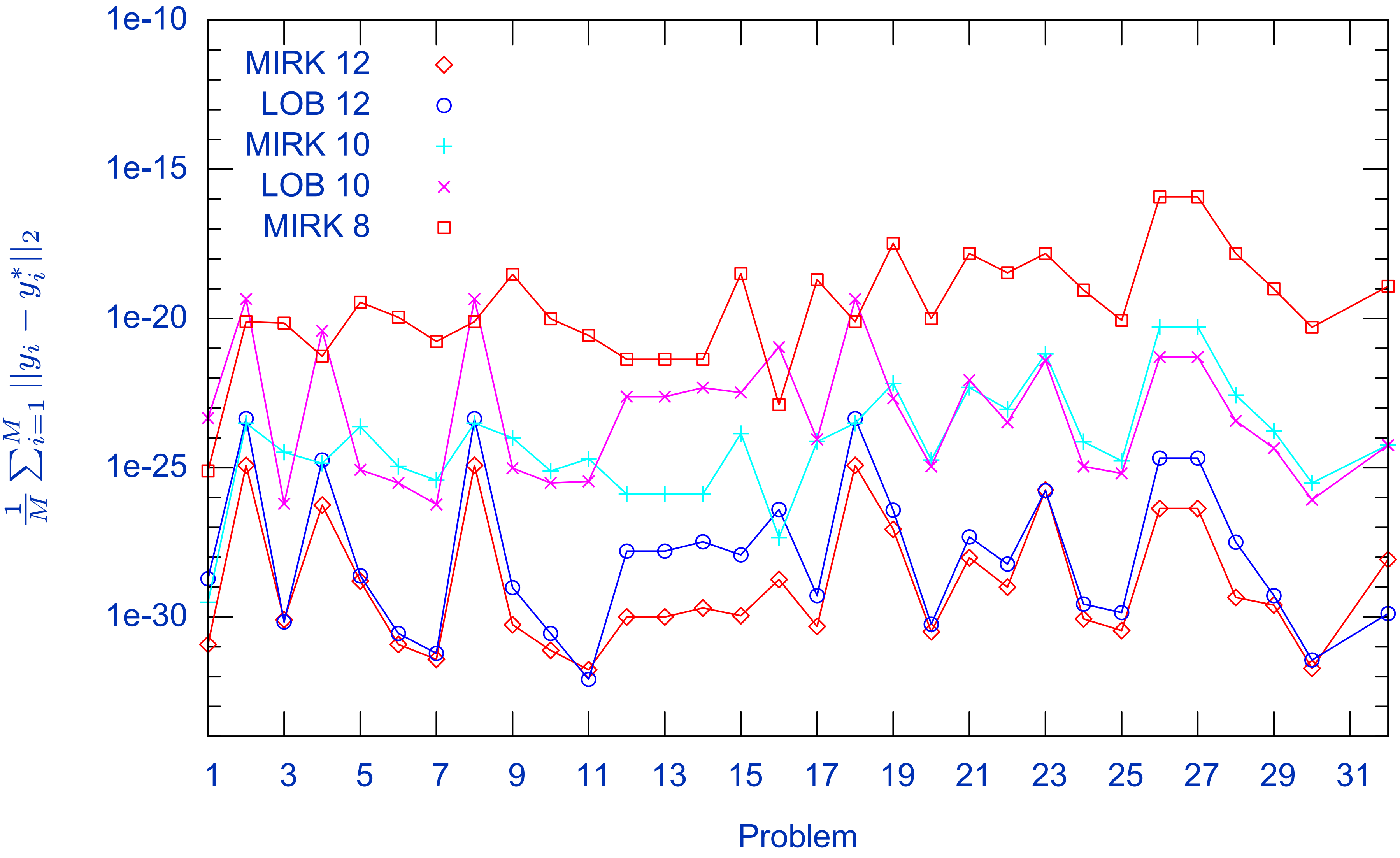
Order	MIRK	LOB
6	3	2
8	7	4
10	14	8
12	24	15

When f is expensive, one would expect the LOB scheme to be considerably quicker than their MIRK counterparts.

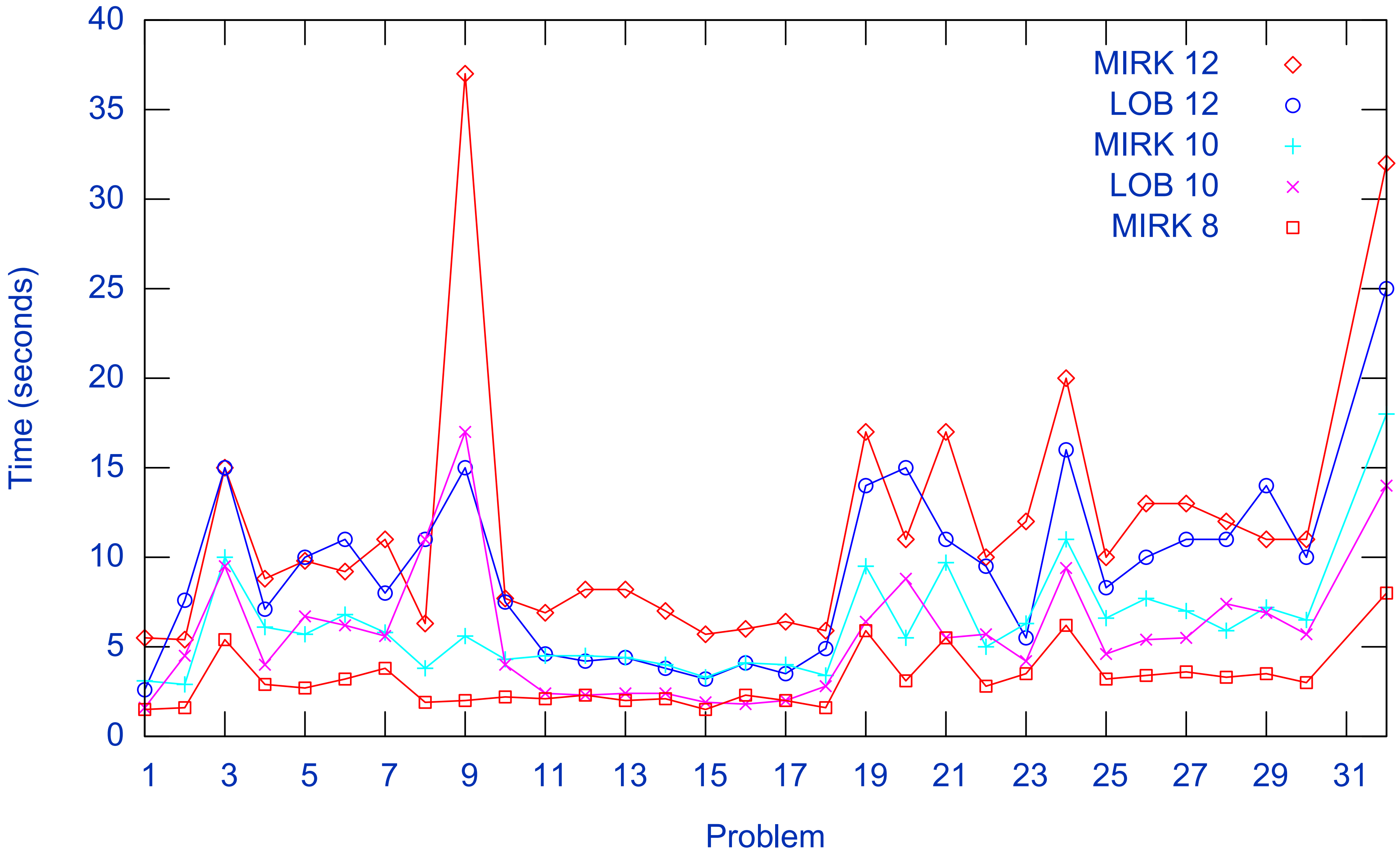
Numerical Tests

- We have developed a Fortran 95 code *NewNRK* with which to test these finite difference schemes.
- 128-bit floating point (≈ 32 decimal digits of accuracy) precision was used.
- We use a test rig of 32 singular perturbation problems, of these, 31 are of the form $y'' = f(x,\ y)$ or $y'' = f(x,\ y,\ y')$.
- A uniform mesh of 1025 points was solved for.

Batch Accuracy



Batch Timing



Results & Conclusions

- LOB 10 is faster and more accurate than MIRK 10 for the majority of the test problems.
- LOB 12 is faster but less accurate than MIRK 12 for the majority of the test problems.
- LOB 12 needs refinement.
- Solutions to $y'' = f(x,\ y)$ problems are computed significantly quicker with LOB than they are with MIRK.

32 test problems

1	$\epsilon y'' - y = 0$	$y(0) = 1,\ \ y(1) = 0.$
2	$\epsilon y'' - y' = 0$	$y(0) = 1,\ \ y(1) = 0.$
3	$\epsilon y'' + (2 + \cos(\pi x))y' - y =$ $-(1 + \epsilon\pi^2)\cos(\pi x) - (2 + \cos(\pi x))\pi \sin(\pi x)$	$y(-1) = y(1) = -1$
4	$\epsilon y'' + y' - (1 + \epsilon)y = 0$	$y(-1) = 1 + \exp(-2)$ $y(1) = 1 + \exp(-2(1 + \epsilon)/\epsilon)$
5	$\epsilon y'' - xy' - y = -(1 + \epsilon\pi^2)\cos(\pi x) + \pi x \sin(\pi x)$	$y(-1) = y(1) = -1$
6	$\epsilon y'' + xy' = -\epsilon\pi^2 \cos(\pi x) - \pi x \sin(\pi x)$	$y(-1) = -2,\ \ y(1) = 0$
7	$\epsilon y'' + xy' - y = -(1 + \epsilon\pi^2)\cos(\pi x) - \pi x \sin(\pi x)$	$y(-1) = -1,\ \ y(1) = 1$
8	$\epsilon y'' + y' = 0$	$y(0) = 1,\ \ y(1) = 2$
9	$(\epsilon + x^2)y'' + 4xy' + 2y = 0$	$y(-1) = y(1) = 1/(1 + \epsilon)$
10	$\epsilon y'' + xy' = 0$	$y(-1) = 0,\ \ y(1) = 2$
11	$\epsilon y'' - y = -(\epsilon\pi^2 + 1)\cos(\pi x)$	$y(-1) = y(1) = -1$
12	$\epsilon y'' - y = -(\epsilon\pi^2 + 1)\cos(\pi x)$	$y(-1) = -1,\ \ y(1) = 0$
13	$\epsilon y'' - y = -(\epsilon\pi^2 + 1)\cos(\pi x)$	$y(-1) = 0,\ \ y(1) = -1$
14	$\epsilon y'' - y = -(\epsilon\pi^2 + 1)\cos(\pi x)$	$y(-1) = y(1) = 0$

32 test problems (2)

15	$\epsilon y'' - xy = 0$	$y(-1) = y(1) = 0$
16	$\epsilon^2 y'' + \pi^2 y/4 = 0$	$y(0) = 0,\ \ y(1) = \sin(\pi/2\epsilon)$
17	$y'' = -3\epsilon y/(\epsilon + x^2)^2$	$y(0.1) = -y(0.1) = 0.1/\sqrt{\epsilon + 0.01}$
18	$\epsilon y'' = -y'$	$y(0) = 1,\ \ y(1) = \exp(-1/\epsilon)$
19	$\epsilon y'' + \exp(y)y' - \frac{\pi}{2}\sin(\pi x/2)\exp(2y) = 0$	$y(0) = y(1) = 0$
20	$\epsilon y'' + (y')^2 = 1$	$y(0) = 1 + \epsilon \ln\cosh(-0.745/\epsilon)$ $y(1) = 1 + \epsilon \ln\cosh(0.255/\epsilon)$
21	$\epsilon y'' = y + y^2 - \exp(-2x/\sqrt{\epsilon})$	$y(0) = 1,\ \ y(1) = \exp(-1/\sqrt{\epsilon})$
22	$\epsilon y'' + y' + y^2 = 0$	$y(0) = 0,\ \ y(1) = \frac{1}{2}$
23	$y'' = \mu \sinh(\mu y)$	$y(0) = 0,\ \ y(1) = 1$
24	$\epsilon A(x) y y'' - \left(\frac{1+\gamma}{2} - \epsilon A'(x)\right) y y' + \frac{y'}{y}$ $+ \frac{A'(x)}{A(x)}\left(1 - \left(\frac{\gamma-1}{2}\right) y^2\right) = 0,$ $A(x) = 1 + x^2,\ \ \gamma = 1.4$	$y(0) = 0.9129,\ \ y(1) = 0.375$
25	$\epsilon y + y y' - y = 0$	$y(0) = -\frac{1}{3},\ \ y(1) = \frac{1}{3}$
26	$\epsilon y + y y' - y = 0$	$y(0) = 1\ \ y(1) = -\frac{1}{3}$
27	$\epsilon y + y y' - y = 0$	$y(0) = 1\ \ y(1) = \frac{1}{3}$

32 test problems (3)

28	$\epsilon y + yy' - y = 0$	$y(0) = 1 \;\; y(1) = \frac{3}{2}$
29	$\epsilon y + yy' - y = 0$	$y(0) = 0 \;\; y(1) = \frac{3}{2}$
30	$\epsilon y + yy' - y = 0$	$y(0) = -\frac{7}{6} \;\; y(1) = \frac{3}{2}$
31	$y' = \sin\theta, \;\; \theta' = M$ $\epsilon M' = -Q, \epsilon Q' = (y-1)\cos\theta - MT$ $T = \sec\theta + \epsilon Q \tan\theta$	$y(0) = y(1) = 0, \;\; M(0) = M(1) = 0$
32	$y'''' = R(y'y'' - yy''')$	$y(0) = y'(0) = 0, \;\; y(1) = 1, \;\; y'(1) = 0$