36th AIAA Fluid Dynamics Conference & Exhibit
05–08 June 2006, San Francisco, CA

AIAA #2006–3064

Generalized Approaches for Constructing Compact Schemes

José A. Camberos*
U.S. Air Force Research Laboratory
Wright–Patterson Air Force Base, Dayton, OH 45433

Larry A. Lambe†
Multidisciplinary Software Systems Research Corporation
Bloomingdale, IL 60108

Three methods found in the literature for deriving compact finite difference schemes will be discussed in this paper. These include (i) An operator is expressed as a series in a difference operator and a Padé approximation of that is taken (Padé methods); (ii) A linear combination of difference operators with unknown coefficients is formed and equations for those coefficients are obtained by matching up corresponding terms in the Taylor series (Taylor series methods); and (iii) Birkhoff interpolation used to to derive relations between function and derivative values at various nodes. The original Padé method appears to go back to the 1950s. The method can also be found in recent books on highaccuracy noncentered compact difference schemes. Taylor series methods were popularized in the 1990s and interpolation methods were presented in a recent paper on the derivation of highorder compact schemes for nonuniform grids. In this paper we use computer aided symbolic computation (SC) to review all three methods. The algebra of difference operators is implemented using ExprLib and all the calculations were done with programs written in ansi c. We note that Taylor series and interpolation methods are suited for deriving schemes on non uniform as well as uniform meshes. Using symbolic computation removes the tedium and tendency for typos for nonuniform methods. We also note that special cases of one method can occur as special cases of others. Our long time goal is to set up an interactive environment for deriving, analyzing, and experimenting with new and known compact schemes in a portable way that allows the developer to reuse code already written regardless of programming language.

Introduction

The past two decades have seen considerable progress on developing high-order, high-resolution accurate schemes for calculating flow fields with shocks. In flow fields containing shock waves, the attention has focused on shock-capturing methods. While first-order accurate schemes are too diffusive, classical central higher-order schemes, which resolve discontinuities better, develop spurious oscillations around regions containing sharp flow discontinuities. Examples include the Lax-Wendroff, Fromm, and Warming-Beam schemes.[1] To capture shocks smoothly, non-oscillatory dissipative schemes with high resolution were developed.

A broad range of physical phenomena contain a wide range of time and length scales (e.g., turbulent flows). Direct numerical simulations of these resolve all the relevant scales in numerical calculations. The accuracy requirement in direct numerical simulations, and large- eddy simulations, of turbulence, computational electromagnetics, and aeroacoustics has become a pacing item for further development. The total-variation diminishing (TVD) and other such schemes are widely used for capturing shock waves accurately. More robust schemes such as essentially non-oscillatory (ENO), weighted-ENO and subsequent schemes have been proposed for improved resolution of shocks and contact discontinuities. For all such schemes, a higher order of accuracy requires a greater number of discrete points, which makes treatment of the boundary conditions difficult, making it impossible to keep the same order of accuracy at the boundary.

To keep the point-stencil small, so-called compact (or Padé) schemes have been well-explored and developed. Compact schemes consider approximate relations between a function and its derivatives at discrete nearby points. Finite difference schemes may be classified as "explicit" or "implicit." Explicit schemes contain only one unknown and the nodal derivatives are expressed directly as a weighted sum of the point values of the function. Implicit

*Aerospace Engineer and AIAA Associate Fellow (jose.camberos@wpafb.af.mil)
†Chief Scientist, MSSRC (llambe@mssrc.com)

schemes contain more than one unknown. Compact schemes are implicit. They equate a weighted sum of the point derivatives to a weighted sum of the function. Such schemes are significantly more accurate for small scales than explicit schemes with the same stencil width. This increase in accuracy is achieved at the cost of inverting a banded (usually tridiagonal) matrix to obtain the nodal derivatives. Since tridiagonal matrices can be inverted very efficiently, compact schemes of this form are extremely attractive when explicit time advance is used.

The essential method behind compact schemes has been known for a long time, as noted by Collatz,[2] although only recently has it been applied in context of fluid flow. Hirsh[?] pioneered such an application for the viscous, incompressible Navier-Stokes equations. In the early 1990s Lele[3] developed central compact finite difference schemes, which perform better than the standard finite-difference approximations. These schemes can be used not only for the evaluation of derivatives, but also for filtering and interpolation to achieve good numerical solutions with very low numerical dissipation. Mahesh[4] has also recently introduced strategy for generating a family of finite difference schemes for first and second derivatives of smooth functions using a coupled-derivative technique. Gaitonde and Shang[?] and Kobayashi[?] proposed and analyzed finite-volume compact schemes. Shukla and Zhong use Birkhoff interpolation to derive compact schemes on non-uniform grids.[5] A good recent history of the use of compact schemes is contained in the Introduction of the paper just cited.

The application of centered compact schemes to compressible flows initially was difficult because of the lack of numerical dissipation intrinsic to centered finite-differences. Filtering mentioned above adds a small amount of dissipation making the schemes stable and practical. Halt[?] noted that the development of compact schemes should investigate the possibility of implementing a non-oscillatory, shock-capturing method, prompting many to propose a variety of upwind compact schemes.[?]

Using symbolic computation (SC), three methods found in the literature for deriving compact finite difference schemes will be revisited in this paper. They proceed as follows.

1. An operator is expressed as a series in a difference operator and a Padé approximation of that is taken (Padé methods).
2. A linear combination of difference operators with unknown coefficients is formed and equations for those coefficients are obtained by matching up corresponding terms in the Taylor series (Taylor series methods).
3. Birkhoff interpolation[6,7] is used to to derive relations between function and derivative values at various nodes.

The original Padé method goes back to Kopal [8, Bibliographical Notes IX–D, p. 520] in the 1950s. The method can also be found, e.g., in [9, §2.6 and §3.2.1]. Taylor series methods can be found in, e.g,[3] and.[4] Interpolation methods are found in.[5]

Rational Approximations to an Operator

Difference Operator Algebra

In order to discuss Padé methods, the difference operator algebra[1,8] must be recalled.

Let $\mathcal{F}$ be the space of real valued functions defined and smooth on all of $\mathbb{R}$. For $f \in \mathcal{F}$, the following *backward*, *forward*, *central*, and *averaging* operators on $\mathcal{F}$.

$$(\Delta(h)(f))(x) = f(x+h) - f(x) \tag{1}$$
$$(\nabla(h)(f))(x) = f(x) - f(x-h) \tag{2}$$
$$(\delta(h)(f))(x) = f\left(x+\frac{h}{2}\right) - f\left(x-\frac{h}{2}\right) \tag{3}$$
$$(\mu(h)(f))(x) = \frac{1}{2}\left(f\left(x+\frac{h}{2}\right) + f\left(x-\frac{h}{2}\right)\right) \tag{4}$$

where $h \in \mathbb{R}$. We call these operators the *basic* difference operators. Note that the objects Δ, ∇, δ, and μ are actually paths in the space of all operators on the function space $\mathcal{F}$. Such paths are added, subtracted, and multiplied in the obvious way:

$$(((\alpha \pm \beta)(h))(f))(x) = (\alpha(h)(f) \pm \beta(h)(f))(x) = \alpha(h)(f)(x) \pm \beta(h)(f)(x) \tag{5}$$
$$(((\alpha\beta)(h))(f))(x) = \alpha(h)(\beta(h)(f))(x). \tag{6}$$

Of course, once the rules are known for the operations in this *operator path algebra* $\mathcal{P}$ are known, a more colloquial notation may be used to calculate in this algebra. This also follows Kopal. For example, we calculate

$$\Delta\nabla f(x) = \Delta(f(x) - f(x-h)) = \tag{7}$$

$$f(x+h) - f(x) - (f(x) - f(x-h)) = f(x+h) - 2f(x) - f(x-h) \tag{8}$$
$$\nabla\Delta f(x) = \nabla(f(x+h) - f(x) - (f(x) - f(x-h)) \tag{9}$$
$$= f(x+h) - 2f(x) + f(x+h) \tag{10}$$

so that Δ and ∇ commute. Now note that

$$(\Delta - \nabla)f(x) = f(x+h) - 2f(x) + f(x-h) \tag{11}$$

so that

$$\Delta\nabla = \Delta - \nabla \tag{12}$$

and from this it follows that if we denote the identity in $\mathcal{P}$ by I (the constant path that maps to the identity operator), we have

$$(I - \nabla)(I + \Delta) = (I + \Delta)(I - \nabla) = I + \Delta - \nabla - \Delta\nabla = I. \tag{13}$$

Thus we have proven the

Lemma 1

$$I + \Delta = (I - \nabla)^{-1}. \tag{14}$$

All of the above can be done *locally* about a fixed point x_i which we call the *base point.* In this context, write

$$f_{i+k} = f(x_i + kh) \tag{15}$$

for $k = m/2$, where m is a non-negative integer. In the following, we will omit the subscript i on x, but we will continue to write $f_{i+k} = f(x + kh)$. The main thing to note is that if p is any algebraic combination of the basic difference operators then

$$p(f) = a_{-k}f_{i-k} + a_{-k+1}f_{i-k-1} + \ldots + a_0 f_i + \ldots + a_{l-1}f_{i+l-1} + a_l f_{i+l} \tag{16}$$

for some constants $a_{-k}, \ldots, a_l$.

The path operator algebra was implemented using ExprLib[10–16] and this was used to perform all relevant calculations in this paper.

Padé Methods

The idea is to approximate an operator E by a Taylor series in some difference operator. Taking a Padé approximation $\frac{p}{q}$ of the series, we have

$$E(f) \approx \frac{p}{q}(f). \tag{17}$$

Multiplying through by q gives $q(E(f)) \approx p(f)$. If E is linear, this is equivalent to the equation

$$QE(f) = PF \tag{18}$$

where F is the matrix

$$F = \begin{bmatrix} f_{i-k} \\ f_{i-k-1} \\ \vdots \\ f_i \\ \vdots \\ f_{i+l-1} \\ f_{i+l} \end{bmatrix}. \tag{19}$$

This gives the approximation

$$E(f) \approx Q^{-1}PF. \tag{20}$$

Kopal's Approximations

Kopal's[8] derivation of rational approximations to the operators $\frac{\partial^k}{\partial x^k}$ will be reviewed in this Section.

Assume that the function f has a convergent Taylor series expansion

$$f(x+h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} h^n \tag{21}$$

about the base point. Kopal makes the interesting observation that this may be viewed as the application of a path in the algebra above (with the domain suitably restricted) by writing

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(x)}{n!} h^n = (e^{h\frac{\partial}{\partial x}})(f)(x). \tag{22}$$

Let $E(h) = e^{h\frac{\partial}{\partial x}}$ denote this path. The topology in $\mathcal{P}$ is taken to be the one in which limits are defined *pointwise*, e.g. for an operator F,

$$e^F = \sum_{n=0}^{\infty} \frac{F^n}{n!} \tag{23}$$

means that for h, f, and x, one has

$$((e^F(h))(f))(x) = e^{F(h)f(x)} \tag{24}$$

where h, f, and x may have to be suitably restricted (which is exactly what is meant by Equation (21) in general).

Now note that

$$(I+\Delta)f(x) = f(x) + f(x+h) - f(x) = f(x+h) \tag{25}$$

so that by what we've said above and Equation (21), we immediately have

Lemma 2

$$E = I + \Delta = (I - \nabla)^{-1} \tag{26}$$

in $\mathcal{P}$.

Now formally, i.e. without regard to convergence, but with respect to purely algebraic identities, the statement that $E = I + \Delta$ is equivalent to

$$h\frac{\partial}{\partial x} = \log(I+\Delta) \tag{27}$$

since $E = e^{hD}$ where $D = \frac{\partial}{\partial x}$. Note that by definition Equation (27) means the following. Let

$$s_n = \sum_{j=1}^{n} (-1)^{j-1} \frac{\Delta^n}{j}. \tag{28}$$

Then in $\mathcal{P}$, $\lim_{n\to\infty} s_n$ exists.

In fact, using ExprLib, we found the following.

Lemma 3 *Let* $f_i = f(x+ih)$, *for* $i = 0, 1, 2, \ldots$ *and let*

$$s_n = \sum_{j=1}^{n} (-1)^{j-1} \frac{\Delta(h)^j}{j}.$$

Then

$$s_n = a_n f_n + \ldots + a_1 f_1 + a_0 f_0 \tag{29}$$

where the coefficients a_i *satisfy*

$$\begin{aligned}
a_n + a_{n-1} + \ldots a_0 &= 0 && (30)\\
na_n + (n-1)a_{n-1} + 2a_2 + \ldots + a_1 &= 1 && (31)\\
n^2 a_n + (n-1)^2 a_{n-1} + 2^2 a_2 + \ldots + a_1 &= 0 && (32)\\
&\vdots && (33)\\
n^n a_n + (n-1)^n a_{n-1} + 2^n a_2 + \ldots + a_1 &= 0. && (34)
\end{aligned}$$

The coefficient matrix of this $(n+1)\times(n+1)$ *system of linear equations is non-singular and hence the* a_i *are uniquely determined by these equations.*

For example, for $n = 3$, the matrix equation is

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 1 & 4 & 9 \\ 0 & 1 & 8 & 27 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}. \tag{35}$$

The coefficient matrix has inverse

$$\begin{bmatrix} 1 & -\frac{11}{6} & 1 & -\frac{1}{6} \\ 0 & 3 & -\frac{5}{2} & \frac{1}{2} \\ 0 & -\frac{3}{2} & 2 & -\frac{1}{2} \\ 0 & \frac{1}{3} & -\frac{1}{2} & \frac{1}{6} \end{bmatrix} \tag{36}$$

Thus, $a_0 = -\frac{11}{6}$, $a_1 = 3$, $a_2 = -\frac{3}{2}$, and $a_3 = \frac{1}{3}$.

Once the pattern for the equations above is seen, it is easy to prove the result by induction. As a consequence, we have

Corollary 1

$$h\frac{\partial}{\partial x} = \log(1 + \Delta(h)). \tag{37}$$

The proof is given by observing that, by the lemma above, the coefficient of $f^{(k)}(x)$ is given by the sum

$$n^k a_n + (n-1)^k a_{n-1} + \ldots + 2^k a_2 + a_1 \tag{38}$$

times h^k since

$$f_j = f(x + jh) = \sum_{i=0}^{\infty} \frac{f^{(i)}(x)}{i!} j^i h^i. \tag{39}$$

Thus, by the equations of the lemma, we clearly have that the term $f(x)$ vanishes and the coefficient of $f'(x)$ is just h and all other derivative terms of order less than $n + 1$ vanish, i.e. in the notation of the lemma,

$$\log(1 + \Delta(h)) = \lim_{n \to \infty} s_n = h\frac{\partial}{\partial x}. \tag{40}$$

Kopal observes that the convergence rate for Equation (27) is too slow to be useful even if a Padé approximation is taken and he derives another series with more useful convergence properties using two easily verified identities which we record in the

Lemma 4

$$\mu^2 = 1 + \frac{1}{4}\delta^2 \tag{41}$$

$$E = 1 + \frac{1}{2}\delta^2 + \delta\mu. \tag{42}$$

The objective is to express the differentiation operator in terms of the central differencing operator δ. From above, we can write $E = 1 + \frac{1}{2}\delta^2 + \delta\sqrt{1 + \frac{1}{4}\delta^2}$ and using the fact that

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \tag{43}$$

it can easily be verified that

$$1 + \frac{1}{2}\delta^2 + \delta\sqrt{1 + \frac{1}{4}\delta^2} = e^{2\sinh^{-1}(\frac{\delta}{2})}. \tag{44}$$

Thus, since $E = e^{h\frac{\partial}{\partial x}}$, we have

Lemma 5

$$h\frac{\partial}{\partial x} = 2\sinh^{-1}(\frac{\delta}{2}).$$

A slightly easier derivation that leads to an equivalent result comes from the computation

$$\delta\mu(f_i) = \frac{1}{2}(f_{i+1} - f_{i-1}) \tag{45}$$

along with the identities

$$\begin{aligned} f(x+h) &= e^{h\frac{\partial}{\partial x}}(f) & (46)\\ f(x-h) &= e^{-h\frac{\partial}{\partial x}}(f) & (47) \end{aligned}$$

so that

$$\delta\mu(f_i) = \frac{1}{2}(f_{i+1} - f_{i-1}) = \sinh(h\frac{\partial}{\partial x})(f) \tag{48}$$

and we also have

Lemma 6

$$h\frac{\partial}{\partial x} = \sinh^{-1}(\delta\mu). \tag{49}$$

Note that

$$\begin{aligned} \sinh^{-1}(\delta\mu) &= \sinh^{-1}\left(\delta\sqrt{1+\frac{1}{4}\delta^2}\right) = \delta - \frac{1}{24}\delta^3 + \frac{3}{640}\delta^5 - \frac{5}{7168}\delta^7 + \frac{35}{294912}\delta^9 + \ldots & (50)\\ &= 2\sinh^{-1}\left(\frac{\delta}{2}\right). & (51) \end{aligned}$$

Padé Schemes

Kopal observes that since the series (50) represents an odd function, it is not appropriate for the application of odd derivatives at tabular points (recall Equation (3) above). There is a similar problem for even derivatives. He fixes these problems by writing

$$\begin{aligned} (h\frac{\partial}{\partial x})^{2s+1} &= \frac{1}{\mu}\left(\frac{2}{\delta}\sinh^{-1}\left(\frac{\delta}{2}\right)\right)^{2s+1}\mu\delta^{2s+1} & (52)\\ (h\frac{\partial}{\partial x})^{2s} &= \left(\frac{2}{\delta}\sinh^{-1}\left(\frac{\delta}{2}\right)\right)^{2s}\delta^{2s} & (53) \end{aligned}$$

(exactly the same series is obtained using $\sinh^{-1}(\delta\mu)$ of course). We have

$$\frac{2}{\delta}\sinh^{-1}\left(\frac{\delta}{2}\right) = 1 - \frac{1}{24}\delta^2 + \frac{3}{640}\delta^4 - \frac{5}{7168}\delta^6 + \frac{35}{294912}\delta^8 - \frac{63}{2883584}x^{10} + \ldots \tag{54}$$

and

$$\frac{1}{\sqrt{1+\frac{\delta^2}{4}}}\left(\frac{2}{\delta}\sinh^{-1}\left(\frac{\delta}{2}\right)\right) = 1 - \frac{\delta^2}{6} + \frac{\delta^4}{30} + \frac{x^6}{140} + \frac{x^8}{630} + \frac{x^{10}}{2772} + \ldots \tag{55}$$

Taking some Padé approximations for (54), we obtain $(1,2)$-approximation

$$\frac{24}{\delta^2+24}, \tag{56}$$

$(2,2)$-approximation

$$\frac{17\delta^2+240}{27\delta^2+240}, \tag{57}$$

and $(4,4)$-approximation

$$\frac{69049\delta^4+2871120\delta^2+14757120}{145125\delta^4+3486000\delta^2+14757120}. \tag{58}$$

For the series (55), we obtain $(1,2)$-approximation

$$\frac{6}{\delta^2+6}, \tag{59}$$

(2, 2)-approximation

$$\frac{\delta^2 + 30}{6\delta^2 + 30}, \tag{60}$$

(4, 4)-approximation

$$\frac{\delta^4 + 105\delta^2 + 630}{15\delta^4 + 210\delta^2 + 630}, \tag{61}$$

and (6, 6)-approximation

$$\frac{5\delta^6 + 1162\delta^4 + 17710\delta^2 + 60060}{140\delta^6 + 3780\delta^4 + 27720\delta^2 + 60060}. \tag{62}$$

These all give rise to *compact* schemes. For example, using the (1, 2)-approximation (59) gives.

$$h\frac{\partial}{\partial x} \approx \frac{6}{\delta^2 + 6}\mu\delta \tag{63}$$

and this yields

$$6\mu\delta(f_i) \approx (\delta^2 + 6)(hf_i'). \tag{64}$$

Expanding terms gives

$$3(f_{i+1} - f_{i-1}) = h(f_{i+1}' - 2f_i' + f_{i-1}' + 6f_i'). \tag{65}$$

which we rewrite as

$$\frac{1}{4}f_{i+1}' + f_i' + \frac{1}{4}f_{i-1}' = \frac{3}{4}\frac{(f_{i+1} - f_{i-1})}{h}. \tag{66}$$

In a similar manner, using the (2, 2) approximation (60) yields the scheme

$$\frac{1}{36h}(f_{i+2} - f_{i-2}) + \frac{14}{18h}(f_{i+1} - f_{i-1}) = \frac{1}{3}f_{i+1}' + f_i + \frac{1}{3}f_{i-1}' \tag{67}$$

which we rewrite as

$$\frac{1}{3}f_{i+1}' + f_i' + \frac{1}{3}f_{i+1}' = \frac{1}{9}\frac{f_{i+2} - f_{i-2}}{4h} + \frac{14}{9}\frac{f_{i+1} - f_{i-1}}{2h}. \tag{68}$$

Finally, using the (4, 4) approximation (61), we derive the scheme

$$\frac{f_{i+3} - f_{i-3}}{2} + 101\frac{f_{i+2} - f_{i-2}}{2} + 425\frac{f_{i+1} - f_{i-1}}{2} = 15f_{i+2}' + 150f_{i+1}' + 300f_i' + 15f_{i-1} + 15f_{i-2} \tag{69}$$

which we rewrite as

$$\frac{1}{20}f_{i+2}' + \frac{1}{2}f_{i+1}' + f_i' + \frac{1}{2}f_{i-1}' + \frac{1}{20}f_{i-2}' = \frac{1}{100}\frac{f_{i+3} - f_{i-3}}{6h} + \frac{101}{150}\frac{f_{i+2} - f_{i-2}}{4h} + \frac{17}{12}\frac{f_{i+1} - f_{i-1}}{2h}. \tag{70}$$

It is interesting to note that if we set $u(x) = \int_a^x f(x)dx$, then equation (66) gives precisely

$$\int_{x-h}^{x+h} f(z)dz = u_{i+1} - u_{i-1} = \frac{h}{3}(f_{i+1} + 4f_i + f_{i-1}) \tag{71}$$

which is Simpson's rule.

Taylor Series Methods

Lele's Family of Schemes

Consider the equations

$$f(x + kh) = \sum_{n=0}^{\infty} k^n \frac{f^{(n)}(x)}{n!}h^n, \quad f(x - kh) = \sum_{n=0}^{\infty}(-1)^n k^n \frac{f^{(n)}(x)}{n!}h^n. \tag{72}$$

Since

$$1 - (-1)^n = \begin{cases} 0, & n \text{ even} \\ 2, & n \text{ odd} \end{cases} \tag{73}$$

we have

$$f(x + kh) - f(x - kh) = \sum_{n=0}^{\infty} \frac{2k^{2n+1}}{(2n+1)!} f^{(2n+1)}h^{2n+1}. \tag{74}$$

Similarly,

$$f'(x+kh) = \sum_{n=0}^{\infty} k^n \frac{f^{(n+1)}(x)}{n!} h^n, \quad f'(x-kh) = \sum_{n=0}^{\infty} (-1)^n k^n \frac{f^{(n+1)}(x)}{n!} h^n \tag{75}$$

so that

$$f'(x+kh) + f'(x-kh) = \sum_{n=0}^{\infty} \frac{2k^{2n}}{(2n)!} f^{(2n+1)} h^{2n}. \tag{76}$$

Setting

$$\phi_k = \frac{f(x+kh) - f(x-kh)}{2kh} = \sum_{n=0}^{\infty} \frac{k^{2n}}{(2n+1)!} f^{(2n+1)}(x) h^{2n} \tag{77}$$

$$\tilde{\phi_k} = f'(x+kh) + f'(x-kh) = \sum_{n=0}^{\infty} \frac{2k^{2n}}{(2n)!} f^{(2n+1)} h^{2n}, \tag{78}$$

Lele[3] considers the equation

$$\frac{1}{2}\tilde{\phi}_0 + \alpha\tilde{\phi}_1 + \beta\tilde{\phi}_2 = a\phi_1 + b\phi_2 + c\phi_3 \tag{79}$$

which, using the notation established above, amounts to

$$\alpha(f'_{i+1} + f'_{i-1}) + f'_i + \beta(f'_{i+2} + f'_{i-2}) = a\frac{f_{i+1} - f_{i-1}}{2h} + b\frac{f_{i+2} - f_{i-2}}{4h} + c\frac{f_{i+3} - f_{i-3}}{6h}. \tag{80}$$

Consider the coefficient of $f^{(2n+1)}h^{2n}$. For $n = 0$, we have

$$1 + 2\alpha + 2\beta = a + b + c, \tag{81}$$

while for $n \geq 1$,

$$\alpha\frac{2}{(2n)!} + \beta\frac{2(2)^{2n}}{(2n)!} = a\frac{1}{(2n+1)!} + b\frac{2^{2n}}{(2n+1)!} + c\frac{3^{2n}}{(2n+1)!}. \tag{82}$$

Clearing denominators gives

$$2(2n+1)(\alpha + 2^{2n}\beta) = a + 2^{2n}b + 3^{2n}c \tag{83}$$

which are the relations derived in.[3] Consider the first six equations

$$a + b + c - 2\alpha - 2\beta - 1 = 0 \tag{84}$$

$$a + 2^{2n}b + 3^{2n}c - 2(2n+1)(\alpha + 2^n\beta) = 0, \; n = 1 \ldots 5. \tag{85}$$

We obtain the following normal forms for the equations giving fourth order schemes

$$a = \frac{2}{3}\alpha - \frac{16}{3}\beta + \frac{5}{3}c + \frac{4}{3} \tag{86}$$

$$b = \frac{4}{3}\alpha + \frac{22}{3}\beta - \frac{8}{3}c - \frac{1}{3} \tag{87}$$

sixth order schemes

$$a = \frac{1}{6}\alpha - \frac{10}{3}\beta + \frac{3}{2} \tag{88}$$

$$b = \frac{32}{15}\alpha + \frac{62}{15}\beta - \frac{3}{5} \tag{89}$$

$$c = -\frac{3}{10}\alpha\frac{6}{5}\beta + \frac{1}{10}, \tag{90}$$

eighth order schemes

$$a = -\frac{7}{6}\alpha + 2 \tag{91}$$

$$b = \frac{284}{75}\alpha - \frac{61}{50} \tag{92}$$

$$c = \frac{9}{50}\alpha - \frac{2}{25} \tag{93}$$

$$\beta = \frac{2}{5}\alpha - \frac{3}{20}, \tag{94}$$

and a unique tenth order scheme

$$a = \frac{17}{12},\ b = \frac{101}{150},\ c = \frac{1}{100},\ \alpha = \frac{1}{2},\ \beta = \frac{1}{20}. \tag{95}$$

Adding on the equation for $n = 5$ results in an inconsistent system, i.e. there are no higher order schemes using this particular stencil.

Note that the scheme given by (95) is exactly the same as the one given by the $(4,4)$-scheme (70).

Another Family of Schemes

In,[4] the following family is considered.

$$a_1 f'(x-h) + a_0 f'(x) + a_2 f'(x+h) + h(b_1 f''(x-h) + b_0 f''(x) + b_2 f''(x+h)) \quad = \tag{96}$$

$$\frac{1}{h}(c_1 f(x-2h) + c_2 f(x-h) + c_0 f(x) + c_3 f(x+h) + c_4 f(x+2h)). \tag{97}$$

Interpolation Methods

Suppose the points $x_1 < x_2 < x_3$ are given and we have values $f_1,\ f_2,\ f_3,\ f_1'$, and f_3'. Berkhoff-Hermite interpolation[17] gives a unique polynomial

$$p(x) = p_4 x^4 + p_3 x^3 + p_2 x^2 + p_1 x + p_0 \tag{98}$$

of degree four, in this case, interpolating the given data. As with all interpolation problems, we can get this polynomial by setting up a generalized Vandermond linear system, viz.

$$p_4 x_1^4 + p_3 x_1^3 + p_2 x_1^2 + p_1 x_1 + p_0 \quad = \quad f_1 \tag{99}$$

$$p_4 x_2^4 + p_3 x_2^3 + p_2 x_2^2 + p_1 x_2 + p_0 \quad = \quad f_2 \tag{100}$$

$$p_4 x_3^4 + p_3 x_3^3 + p_2 x_3^2 + p_1 x_3 + p_0 \quad = \quad f_3 \tag{101}$$

$$4p_4 x_1^3 + 3p_3 x_1^2 + 2p_2 x_1 + p_1 \quad = \quad f_1' \tag{102}$$

$$4p_4 x_3^3 + 3p_3 x_3^2 + 2p_2 x_3 + p_1 \quad = \quad f_3' \tag{103}$$

which is the system

$$\begin{bmatrix} x_1^4 & x_1^3 & x_1^2 & x_1 & 1 \\ x_2^4 & x_2^3 & x_2^2 & x_2 & 1 \\ x_3^4 & x_3^3 & x_3^2 & x_3 & 1 \\ 4x_1^3 & 3x_1^2 & 2x_1 & 1 & 0 \\ 4x_3^3 & 3x_3^2 & 2x_3 & 1 & 0 \end{bmatrix} \begin{bmatrix} p_4 \\ p_3 \\ p_2 \\ p_1 \\ p_0 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_1' \\ f_3' \end{bmatrix}. \tag{104}$$

Assuming that $x_1 = a - h$, $x_2 = a$, and $x_3 = a + h$, for $h \neq 0$, since the coefficient matrix has determinant (as computed using ExprLib) $16h^8$ there is indeed a unique solution to the above equation which is a linear combination of the $f_1,\ f_2,\ f_3,\ f_1'$, and f_3'. Since p does not interpolate f_2' at x_2, we can obtain a relation using $p'(x_2)$. In fact, using ExprLib, we find that

$$f_2' = p'(x_2) = -\frac{1}{4}\left(f_1' + f_3'\right) + \frac{3}{4h}\left(f_3 - f_1\right). \tag{105}$$

Setting $a = x_i$ and $f_1 = f_{i-1} = f(x-h)$, $f_i = f(x_i)$, etc. gives

$$\frac{1}{4} f_{i-1}' + f_i' + \frac{1}{4} f_{i+1}' = \frac{3}{4h}\left(f_{i+1} - f_{i-1}\right) \tag{106}$$

which recovers the $(1,2)$-Padé and the special case of Lele's one parameters family scheme from the Sections above.

Formulas were derived for $(0,1)$-interpolation in[5] and used to derive schemes for non-uniform meshes, however the current approach simply uses symbolic computation on a computer (ExprLib) to derive such formulas. For example, using $x_1 = x_{i-1}$, $x_2 = x_i$, and $x_3 = x_{i+1}$ in a matter of a fraction of a second, we obtain the relation

$$c_1 f_{i-1}' + c_2 f_i' + c_2 f_{i+1}' = a_1 f_{i-1} + a_2 f_i + a_3 f_{i+1} \tag{107}$$

where

$$c_1 = (x_{i+1} - x_{i-1})x_{i+1}^4 + (-3x_{i+1}^2 + 2x_{i-1}x_i + x_{i-1}^2)x_{i+1}^3 + (3x_{i+1}^3 - 3x_{i-1}x_i)x_{i+1}^2 + \tag{108}$$
$$(-x_i^4 - 2x_{i-1}x_i^3 + 3x_{i-1}^2 x_{i+1}^2)x_{i+1} + x_{i-1}x_i^4 - x_{i-1}^2 x_i^3 \tag{109}$$
$$c_2 = (x_i - x_{i-1})x_{i+1}^4 + (-x_i^2 - 2x_{i-1}x_i + 3x_{i-1}^2)x_{i+1}^3 + (3x_{i-1}x_i^2 - 3xi - 1^3)x_{i+1}^2 + \tag{110}$$
$$(-3x_{i-1}^2 x_{i+1}^2 + 2x_{i-1}^3 x_i + x_{i-1}^4)x_{i+1} + x_{i-1}^3 x_i^2 - x_{i-1}^4 x_i \tag{111}$$
$$c_3 = (x_i^3 - 3x_{i-1}x_i^2 + 3x_{i-1}^2 x_i - x_{i-1}^3)x_{i+1}^2 + (-x_i^2 + 2x_{i-1}x_i^3 - 2x_{i-1}^3 x_i + x_{i-1}^4)_{i+1}x + \tag{112}$$
$$x_{i-1}x_i^4 - 3x_{i-1}^2 x_i^3 + 3x_{i-1}^3 x_i^2 - x_{i-1}^4 x_i \tag{113}$$

and

$$-a_1 = 2x_{i+1}^4 + (-4x_{i+1} - 4x_{i-1})x_{i+1}^3 + 12x_{i-1}x_i x_{i+1}^2 + (4x_i^3 - 12x_{i-1}x_i^2)x_{i+1} - \tag{114}$$
$$2x_i^4 + 4x_{i-1}x_i^3 \tag{115}$$
$$-a_2 = -2x_{i+1}^4 + (4x_i + 4xi - 1)x_{i+1}^3 - 12x_{i-1}x_i x_{i+1}^2 + (12xi - 1^2 x_i - 4x_{i-1}^3)x_{i+1} - \tag{116}$$
$$4x_{i-1}^3 x_i + 2xi - 1^4 \tag{117}$$
$$-a_3 = (-4x_i^2 + 12x_{i-1}x_i^2 - 12x_{i-1}^2 x_i + 4x_{i-1}^3)x_{i+1} + 2x_i^4 - 4x_{i-1}x_i^3 + 4x_{i-1}^3 x_i - 2x_{i-1}^4. \tag{118}$$

It is interesting to note that when $x_{i-1} = a - h$, $x_i = a$, and $x_{i+1} = a + h$, $a_2 = 0$, and we obtain equation (106) as we should.

Conclusions

Acknowledgments

The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of Air Force Research Laboratory, Department of Defense, or the U.S. Government.

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[16] See <www.mssrc.com> for further examples.

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