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# LIP: The Livermore Interpolation Package, Version 1.3

F. N. Fritsch

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# The Livermore Interpolation Package

Version 1.3

Frederick N. Fritsch

Physical and Life Sciences Directorate
Condensed Matter & Materials Division

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# Contents

# Introduction

This report describes LIP, the Livermore Interpolation Package. Because LIP is a stand-alone version of the interpolation package in the Livermore Equation of State (LEOS) access library, the initials LIP alternatively stand for the "LEOS Interpolation Package". LIP was totally rewritten from the package described in [1]. In particular, the independent variables are now referred to as x and y, since the package need not be restricted to equation of state data, which uses variables ρ (density) and T (temperature).

LIP is primarily concerned with the interpolation of two-dimensional data on a rectangular mesh. The interpolation methods provided include piecewise bilinear, reduced (12-term) bicubic, and bicubic Hermite (biherm). There is a monotonicity-preserving variant of the latter, known as bimond. For historical reasons, there is also a biquadratic interpolator, but this option is not recommended for general use. A birational method was added at version 1.3. In addition to direct interpolation of two-dimensional data, LIP includes a facility for inverse interpolation (at present, only in the second independent variable). For completeness, however, the package also supports a compatible one-dimensional interpolation capability. Parametric interpolation of points on a two-dimensional curve can be accomplished by treating the components as a pair of one-dimensional functions with a common independent variable.

LIP has an object-oriented design, but it is implemented in ANSI Standard C for efficiency and compatibility with existing applications. First, a "LIP interpolation object' is created and initialized with the data to be interpolated. Then the interpolation coefficients for the selected method are computed and added to the object. Since version 1.1, LIP has options to instead estimate derivative values or merely store data in the object. (These are referred to as "partial setup" options.) It is then possible to pass the object to functions that interpolate or invert the interpolant at an arbitrary number of points.

The first section of this report describes the overall design of the package, including both forward and inverse interpolation. Sections 2–6 describe each interpolation method in detail. The software that implements this design is summarized function-by-function in Section 7. For a complete example of package usage, refer to Section 8. The report concludes with a few brief notes on possible software enhancements. For guidance on adding other functional forms to LIP, refer to Appendix B.

The reader who is primarily interested in using LIP to solve a problem should skim Section 1, then skip to Sections 7.1–4. Finally, jump ahead to Section 8 and study the example. The remaining sections can be referred to in case more details are desired.

Changes since version 1.1 of this document include the new Section 3.2.1 that discusses derivative estimation and new Section 6 that discusses the birational interpolation method. Section numbers following the latter have been modified accordingly. (Note that version 1.2 was not formally documented.)

# 1. Overall Package Design

This section describes the overall design of LIP. The organization of the software that implements this design is described in Section 7, below.

### *1.1. Data*

Throughout this report we assume that data has been given for some function f(x,y) on a rectangular mesh $\mathbf{x} = (x_0, x_1, ..., x_{nx-1})$, $\mathbf{y} = (y_0, y_1, ..., y_{ny-1})$. Subscripting is from zero to be consistent with the C code. The data values are $f_{ij} = f(x_i,y_j)$. There are nx×ny data values, (nx–1)×(ny–1) mesh rectangles (boxes). The mesh is arbitrary, except that we require:

$$x_{i-1} < x_i, \qquad i = 1, \ldots, nx-1; \tag{1.1x}$$

$$y_{j-1} < y_j, \qquad j = 1, \ldots, ny-1. \tag{1.1y}$$

In the C code, the data array is one-dimensional, with `data[j*nx+i]` = $f(x_i,y_j)$.

### *1.2. Compatible univariate interpolation*

The motivation for including univariate interpolation in the original LEOS access library was to handle the univariate "cold curves" that are provided by LEOS. For a compatible interpolation method, it is expected that

$$Ft = Fc + Fe + Fi\ , \tag{1.2}$$

where the second letters stand for total (t), cold (c), electronic (e) and ionic (i). Fc is univariate (a function of density only), and the others are bivariate. (Here F = E or P.) The univariate interpolant needs to be compatible with its bivariate interpolant of the same type (bilinear, bicubic, or biherm), in the sense that if the data for these four functions satisfy (1.2), then so will the interpolants (to as close to machine precision as possible).

The current package contains compatible linear, cubic, and cubic Hermite interpolators. Since the EOP data is available only for Ft, there is no univariate quadratic interpolator.

In the case of univariate data supported by LIP, one of the independent variables is omitted, as well as the associated index on the data array. When ny=0, `data[i]` = $f(x_i)$; when nx=0, `data[j]` = $f(y_j)$.

### *1.3. Interpolation coefficients*

After an interpolation object has been initialized, the normal first step is to select an interpolation method and then compute interpolation coefficients for that method. The resulting object is then ready to be used for the desired application. The full coefficient array contains ncoef×nboxes = ncoef×(nx–1)×(ny–1) numbers, where ncoef increases as the smoothness of the interpolation method increases. See the following table.

| Method | ncoef | Function | Derivatives | Monotonic? |
|---|---|---|---|---|
| Bilinear | 4 | Continuous | Jump discontinuity across mesh lines | Yes |
| Biquadratic | 9 | Continuous only at data points | Usually not continuous | No |
| Bicubic | 12 | Continuous (due to changed derivative approximation; see Section 3.2.1) | Continuous along mesh lines; may be discontinuous across mesh lines | No |
| Bicubic Hermite | 16 | Continuous | Continuous across mesh lines | May not be |
| Bimond | 16 | Continuous | Continuous across mesh lines | Yes |

The univariate piecewise linear interpolant requires two coefficients per mesh cell, whereas the univariate cubic interpolants all use ncoef=4.

### *1.4. Partial Setup Options*

The primary new capability of LIP version 1.1 was the provision for partial setup (not requiring the full coefficient array). Full support for partial setup was available in most cases at version 1.2. This has two motivations. First, and foremost, was the desire to reduce the memory requirements, possibly at the expense of reduced evaluation speed. A secondary motivation was the ability to incorporate other interpolation methods that do not fit naturally into the standard interpolation coefficient mold. Note that the birational method added at version 1.3 is such a method.

Three basic modes are available in version 1.1 and subsequent versions:

(1) *Full coefficient setup*. This was the standard mode in version 1.0.

(2) *Derivatives-only setup*. Approximate derivative values; compute coefficients as needed at evaluation time. This comes in two flavors: (2a) first partial derivatives only, or (2b) first derivatives and twists. The latter is relevant only for bicubic Hermite interpolation (see Section 4, below).

(3) *Data-only setup*. Store data and interpolate directly from the data array.

The storage requirements for each mode are as follows, with ncoef as in previous table:

Mode (1) bivariate: ndata + ncoef × (nx–1) × (ny–1)

Mode (1) univariate: ndata + ncoef × max[(nx–1),(ny–1)]

Mode (2a) bivariate: ndata + 2×nx×ny

Mode (2a) univariate: ndata + max(nx,ny)

Mode (2b) bivariate: ndata + 3×nx×ny

Mode (3): ndata

In the above formulas,

ndata = nx×ny + nx + ny, for bivariate data;
ndata = 2×max(nx,ny), for univariate data.

For example, for bicubic Hermite we see that ratio of mode (1) to mode (2a) storage requirements is approximately 17/3=5.66...

At present, not all modes are available for all methods. The following table summarizes the availability in LIP version 1.3.

| **Method** | **dimension** | **Mode (1)** | **Mode(2a)** | **Mode(2b)** | **Mode (3)** |
|---|---|---|---|---|---|
| Bilinear | bivariate | Yes | N/A[1] | N/A[1] | Yes |
| | univariate | Yes | N/A[1] | N/A[1] | Yes |
| Biquadratic | bivariate | Yes | No | No | No |
| Bicubic | bivariate | Yes | Yes[2] | N/A | Yes[2] |
| | univariate | Yes | Yes | N/A | Yes |
| Bicubic Hermite | bivariate | Yes | Yes | Yes | Yes |
| | univariate | Yes | Yes | N/A | Yes |
| Bimond | bivariate | Yes | Yes | Yes | Yes[3] |
| | univariate | Yes | Yes | N/A | No |
| Birational | --- | N/A | N/A | N/A | Yes |

Notes:

1. If a Mode (2) setup is attempted for linear interpolation, Mode (3) results.

2. The two-phase modification (see Secton 3.3) is not done in Mode (2) or (3).
3. It is not guaranteed that the computed function and/or derivative values will be identical to those using other modes.

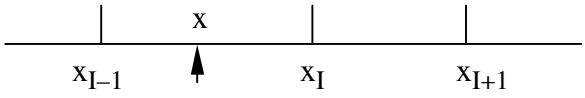
Partial setup (Mode >1) is currently supported for inverse evaluation in all bivariate cases marked "Yes" in the above table, except for bimond.

### *1.5. Forward interpolation (evaluation)*

Given an array of points ($x_{int}$, $y_{int}$) at which interpolation is desired, the first step is to call a table lookup function twice, the first to determine the indices of the $x_{int}$ in **x**, and the second to locate the $y_{int}$ in **y**. This step is independent of the interpolation method.

With any functional form, a nontrivial part of the evaluation for a given (x, y) is determining box indices i and j such that $x_i \le x < x_{i+1}$ and $y_j \le y < y_{j+1}$. The two variables are searched independently. LIP uses a binary search with guess. The index found at one point is saved and used as a guess at the interval index for the next point. (The index for the first point is initialized to zero.) If the defining conditions are already satisfied by the saved index, we are done. If not, the next interval in the direction of the input value is examined. If that test also fails, then a binary search is performed on the remaining part of the data.

For example, let I be the saved x-index. If $x_{I-1} \le x < x_I$, the test $x_I \le x$ will fail. From the direction of the failure, the code will then test for $x_{I-1} \le x$. This succeeds in this case, and the new x-index is i=I–1. If $x < x_{I-1}$, however, a binary search will then be performed in $[x_0, x_{I-1}]$.




In order to provide thread-safety, the function `lip_lookup` that implements the lookup procedure for a single variable saves no state between calls. It does proceed as indicated, but starts anew for each array it is asked to look up. It returns an array of indices, which are then passed on to the appropriate evaluation routine for a most efficient computation.

The mesh index arrays are partitioned into subsets such that all of the consecutive ($x_{int}$, $y_{int}$) lie in the same mesh box ($i_{box}$, $j_{box}$), and the interpolant is evaluated at all of those points using a common set of ncoef interpolation coefficients via a call to `lip_evalu_box`. This, in turn, calls a specific evaluator, which depends on the method. The variables are transformed as indicated below and the interpolation coefficients are obtained. If the full coefficient array is available, a pointer is set to the appropriate location in the coefficient array. If partial setup has been implemented, the coefficients for this mesh box are computed. Then the appropriate equation is evaluated. If derivatives are requested, the appropriate derivative formulas are also evaluated, and the values are returned to the calling program. These evaluators are described in more detail below.

A similar procedure is used in the univariate case, but there is, of course, only a single call to `lip_lookup`. The analog of `lip_evalu_box` is called `lip_evalu_cell`.

### *1.6. Variable transformation*

For the standard bivariate forms, the following variable transformations are used to simplify formulas and enhance numerical stability:

$$x = \text{xscale}(x_{int}) = (x_{int} - x_i) / \Delta x_i, \ \Delta x_i = x_{i+1} - x_i; \qquad (1.3x)$$

$$y = \text{yscale}(y_{int}) = (y_{int} - y_j) / \Delta y_j, \ \Delta y_j = y_{j+1} - y_j. \qquad (1.3y)$$

Here $(x_{int},y_{int})$ is the point in the original variables at which interpolation is desired, and (x,y) is the transformed (scaled) point. Note that these scale functions have the property

$$\text{xscale}(x_i)=0, \ \text{xscale}(x_{i+1})=1, \ \text{yscale}(y_j)=0, \ \text{yscale}(y_{j+1})=1, \qquad (1.4)$$

so that the rectangle $R_{ij}=[x_i,x_{i+1}]\times[y_j,y_{j+1}]$ is mapped onto the unit square $U=[0,1]\times[0,1]$.

These scaling transformations are performed in the method-dependent functions called by `lip_evalu_box`.

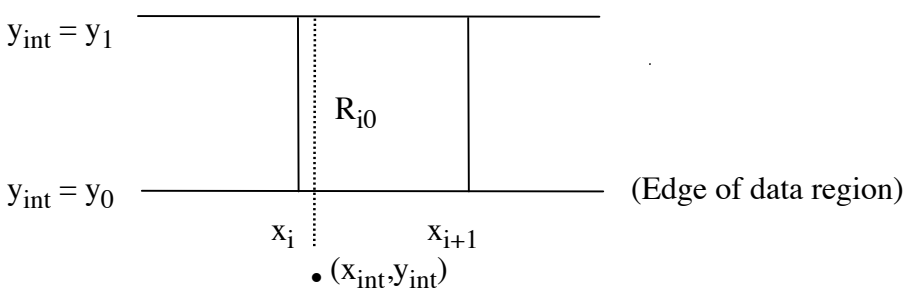
### *1.7. Extrapolation*

If an interpolation point $(x_{int},y_{int})$ is outside the data mesh (i.e., $x_{int} < x_0$ or $x_{int} > x_{nx-1}$, $y_{int} < y_0$ or $y_{int} > y_{ny-1}$), we are in an "extrapolation" situation. The current LIP evaluators allow two extrapolation options, controlled by argument `extr_flag`.

If `extr_flag=0` and $(x_{int},y_{int})$ is outside the table, then the value at the nearest boundary point is returned. (That is, no extrapolation is performed.) If derivatives are requested, zero is returned to match the constant behavior of the extrapolant.

On the other hand, if `extr_flag=1` and $(x_{int},y_{int})$ is outside the table, the value of the function and derivative at the nearest edge point are computed. The linear function determined by these two values is evaluated at $(x_{int},y_{int})$ for the returned value. (This will be linear in the out-of-range variable and the order requested in the other.) The edge derivatives are returned if requested. If both values are out of range, then the bilinear extrapolant determined by the function and derivative values at the nearest corner is used.

As an example, suppose $x_i < x_{int} < x_{i+1}$ but $y_{int} < y_0$ (extrapolation in y):



In this case, we will have scaled variable values 0<x<1, but y<0. If `extr_flag=0`, then $f(x_{int},y_0)$, the value at (x,0), will be returned. If `extr_flag=1`, then $\partial f(x_{int},y_0)/\partial y$ will also be computed (even if not requested) and $f(x_{int},y_0) + (y_{int}-y_0)\ \partial f(x_{int},y_0)/\partial y$ will be returned.

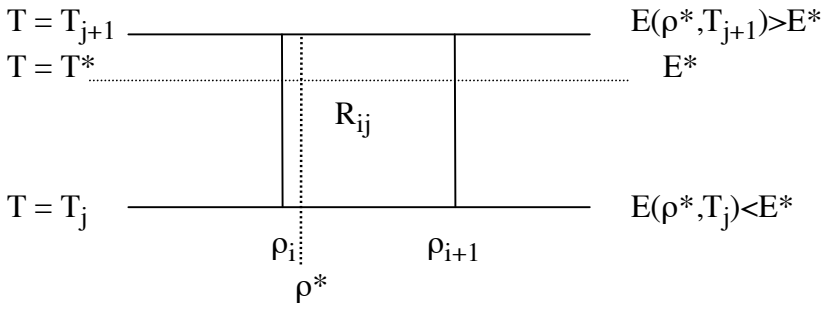
### *1.8. Inverse interpolation*

Many equation of state applications use ρ and E as the fundamental variables. In order to use the LEOS tables, which use (ρ,T) as independent variables, it is necessary to do an inverse lookup. Given values (ρ,E) = (ρ*,E*), we need to find a temperature T=T* such that

$$E(\rho^*,T^*) = E^*. \tag{1.5}$$

The value (ρ*,T*) can then be used as $(x_{int},y_{int})$ in the standard evaluation procedure. This was the original motivation for including an inversion feature in the LEOS interpolation package, and it has been retained in LIP. At present, inversion is only supported in the second independent variable (called T here).

The same lookup procedure described above is used to find i such that $\rho_i \le \rho^* < \rho_{i+1}$. It is then necessary to examine the values $E_j = E(\rho^*,T_j)$, j = 0, 1, ..., ny–1 to find a j such that $E_j \le E^* < E_{j+1}$. A sequential search might require ny evaluations of E to determine j. To reduce code complexity, a simple binary search (without guess) is currently employed. Caution: This assumes that E is monotonic in T; i.e., $E_j < E_{j+1}$, j = 0, ..., ny–2.




We observe that these evaluations are also made simpler by using the fact that $T=T_j$ implies that y=0, and $T=T_{j+1}$ implies that y=1. (But not in the biquadratic case, as discussed in Section 5.3, below.)

At version 1.2, `lip_inverse_vals` was reorganized to support partial setup options. When the full coefficient array is available, `lip_inv_coeff` proceeds as above, using formulas that depend directly on the functional form. At the opposite extreme is `lip_inv_general`, which implements a modified Newton-Raphson iteration and computes new $E(\rho^*,T_j)$ values as needed by calls to `lip_evalu_bivar`. Intermediate between these is `lip_inv_partial`, which computes coefficients for each new box (i, j´) encountered in the above binary search from available information, depending on the setup mode. The new argument `inv_mode` was added to `lip_inverse_vals`

(thus introducing an incompatibility with version 1.1) to control usage of these three sub-functions.

If the input ρ-value is out of range, the above-mentioned inversion is carried out using the appropriate border strip. If the E-value is out of range, the algorithm returns the associated boundary T-value, with zero T-derivative. (There is no linear extrapolation option.)

# 2. Piecewise Bilinear Interpolation

This section describes the bilinear interpolation method as currently supported by LIP.

### *2.1. The bilinear form*

The bilinear functional form on the mesh rectangle $R_{ij}$ is:

$$f(x_{int},y_{int}) = l(x,y) = a_0 + a_1x + a_2y + a_3xy \ , \tag{2.1}$$

where (x,y) are as in (1.3). Once the coefficients $a_k$ have been determined for a given mesh rectangle $R_{ij}$, it is straightforward to evaluate the bilinear form at any $(x_{int},y_{int})$ in the box from (2.1).

### *2.2. Calculating interpolation coefficients*

The interpolation conditions on mesh rectangle $R_{ij}$ are:

$$f_{mn} = f(x_m,y_n), \ m = i, i+1, \ n = j, j+1. \tag{2.2}$$

There are four coefficients in (2.1) and four conditions in (2.2). Using (2.2), we can write down the coefficients immediately from (2.1).

$$f_{ij} = f(x_i,y_j) = l(0,0) = a_0; \tag{2.3a}$$

$$f_{i+1,j} = f(x_{i+1},y_j) = l(1,0) = a_0 + a_1; \tag{2.3b}$$

$$f_{i,j+1} = f(x_i,y_{j+1}) = l(0,1) = a_0 + a_2; \tag{2.3c}$$

$$f_{i+1,j+1} = f(x_{i+1},y_{j+1}) = l(1,1) = a_0 + a_1 + a_2 + a_3. \tag{2.3d}$$

(2.3a) gives us $a_0$ directly:

$$a_0 = f_{ij}. \tag{2.4a}$$

From (2.3b) and (2.4a) we have

$$a_1 = f_{i+1,j} - f_{ij}. \tag{2.4b}$$

Similarly, (2.3c) and (2.4a) yield

$$a_2 = f_{i,j+1} - f_{ij}. \tag{2.4c}$$

Finally, (2.3d) gives us

$$a_3 = f_{i+1,j+1} - (a_0 + a_1 + a_2). \tag{2.4d}$$

We observe that, by construction, the bilinear form will be continuous across the box boundaries. However, derivatives will have jump discontinuities there.

The interpolation coefficients are laid out in blocks of four in memory, with the coefficients for mesh rectangle $R_{ij}$ starting at location `(j*(nx-1)+i)*4` in the coefficient array.

### *2.3. Direct inversion (bilinear)*

Once the appropriate T-interval has been found, as discussed in Section 1.8, we need to solve equation (1.5) for T=T*. In the bilinear case, this is quite simple. From (2.1) we have

$$E(\rho^*,T) = a_0 + a_1 x^* + a_2 y + a_3 x^* y, \tag{2.5}$$

where

$$x^* = (\rho^* - \rho_i) / (\rho_{i+1} - \rho_i).$$

Equation (2.5) can be solved directly for y,

$$y = ( E^* - (a_0 + a_1 x^*) ) / (a_2 + a_3 x^*), \tag{2.6}$$

and the desired value (obtained by inverting (1.3y) with $y_{int} = T$) is:

$$T^* = (T_{j+1} - T_j)\, y + T_j. \tag{2.7}$$

### *2.4. The univariate analog*

The linear functional form on the mesh interval $[x_i, x_{i+1}]$ is:

$$f(x_{int}) \;=\; l(x) \;=\; a_0 + a_1 x, \tag{2.8}$$

where, unlike in (1.3x), we do *not* divide by the interval length:

$$x \;=\; \text{xscale}(x_{int}) \;=\; x_{int} - x_i. \tag{2.9}$$

Since a univariate linear function is uniquely determined by its values at two distinct points, it is easy to compute the linear interpolation coefficients. The linear interpolant on the mesh interval $[x_i, x_{i+1}]$ is thus determined by

$$f_k = f(x_k),\; k = i, i+1. \tag{2.10}$$

Using (2.8) and (2.9), we can write conditions for the coefficients:

$$f_i \;=\; f(x_i) \;=\; l(0) \;=\; a_0; \tag{2.11a}$$

$$f_{i+1} \;=\; f(x_{i+1}) \;=\; l(x_{i+1} - x_i) \;=\; a_0 + a_1 (x_{i+1} - x_i). \tag{2.11b}$$

(2.11a) gives us $a_0$ directly:

$$a_0 = f_i. \tag{2.12a}$$

From (2.11b) and (2.12a) we have

$$a_1 = (f_{i+1} - f_i) / (x_{i+1} - x_i). \tag{2.12b}$$

The same formulas are used, with the obvious change of notation, if the independent variable is y instead of x.

# 3. Piecewise Bicubic Interpolation

This section describes the reduced bicubic interpolation method as currently supported by LIP. This form was inherited from the LEOS interpolation package.

### *3.1. The bicubic form*

The reduced ("LEOS standard") bicubic functional form on the mesh rectangle $R_{ij}$ is:

$$\begin{aligned} f(x_{int},y_{int}) = c(x,y) = {} & a_0 + a_1x + a_2y + a_3xy + \\ & a_4x^2 + a_5x^2y + a_6x^3 + a_7x^3y + \\ & a_8y^2 + a_9xy^2 + a_{10}y^3 + a_{11}xy^3, \end{aligned} \tag{3.1}$$

where the four highest-order terms ($x^2y^2$, $x^3y^2$, $x^2y^3$, $x^3y^3$) have been omitted from the general bicubic polynomial to reduce storage space and evaluation time. Because the first four terms in (3.1) are the same as in (2.1), we note that a bilinear function can be viewed as a bicubic with its last eight coefficients equal to zero.

### *3.2. Calculating interpolation coefficients*

The same four interpolation conditions (2.2) apply to the bicubic form on mesh rectangle $R_{ij}$, but there are twelve coefficients in (3.1), so we must find eight additional equations. If we had the values of the first partial derivatives of f at the data points, we could supplement (2.2) with the eight derivative interpolation conditions:

$$D_xf_{mn} = \partial f(x_m,y_n)/\partial x, \quad m = i, i+1, \; n = j, j+1. \tag{3.2a}$$

$$D_yf_{mn} = \partial f(x_m,y_n)/\partial y, \quad m = i, i+1, \; n = j, j+1. \tag{3.2b}$$

where $D_xf_{mn}$ is the x-derivative of f at the mn data point, and similarly for $D_yf_{mn}$. To approximate the needed derivatives, we bring in information from neighboring points. See Section 3.2.1, below, for details on how this is done.

Requiring the derivatives of bicubic (3.1) to match the two values $D_xf_{ij}$ and $D_xf_{i+1,j}$ in (3.2a) gives two additional equations. Applying this procedure at $y= y_{j+1}$ gives two more. The other four equations are determined similarly, by reversing the roles of x and y and using (3.2b) instead of (3.2a).

Differentiating (3.1), and taking (1.3) into account, gives the partial derivatives required for (3.2a) and (3.2b) in $R_{ij}$:

$$\begin{aligned} \partial f(x_{int},y_{int})/\partial x = \partial c(x,y)/\partial x \,/\, \Delta x_i = {} & [\, a_1 + a_3y + 2a_4x + 2a_5xy + \\ & 3a_6x^2 + 3a_7x^2y + a_9y^2 + a_{11}y^3] \,/\, \Delta x_i. \end{aligned} \tag{3.3a}$$

$$\begin{aligned} \partial f(x_{int},y_{int})/\partial y = \partial c(x,y)/\partial y \,/\, \Delta y_j = {} & [\, a_2 + a_3x + a_5x^2 + a_7x^3 + \\ & 2a_8y + 2a_9xy + 3a_{10}y^2 + 3a_{11}xy^2] \,/\, \Delta y_j. \end{aligned} \tag{3.3b}$$

This leads to a system of 12 linear equations to be solved for the 12 coefficients ($a_0$, $a_1$, …, $a_{11}$) in (3.1). Note that properties (1.4) greatly simplify the matrix setup. In fact, the matrix is constant, independent of the data. It is set up for interpolation on the unit square with the first four rows of the matrix containing the conditions for interpolating the data at the four corners, f(`x[i],y[i]`) = `rhs[i]`, where

```
x[ 0] = 0;  y[ 0] = 0;
x[ 1] = 0;  y[ 1] = 1;
x[ 2] = 1;  y[ 2] = 0;
x[ 3] = 1;  y[ 3] = 1.
```

Rows 4–7 contain x-derivative interpolation conditions, ∂f(`x[i],y[i]`)/∂x = `rhs[i]`, where

```
x[ 4] = 0;  y[ 4] = 0;
x[ 5] = 1;  y[ 5] = 0;
x[ 6] = 0;  y[ 6] = 1;
x[ 7] = 1;  y[ 7] = 1.
```

Rows 8–11 contain y-derivative interpolation conditions, ∂f(`x[i],y[i]`)/∂y = `rhs[i]`, where

```
x[ 8] = 0;  y[ 8] = 0;
x[ 9] = 0;  y[ 9] = 1;
x[10] = 1;  y[10] = 0;
x[11] = 1;  y[11] = 1.
```

Note that the ∂f/∂x conditions are not in the same order as the others. This is because it is natural to generate x-derivative estimates with y constant, y-derivative estimates with x constant.

The resulting constant matrix is (in C notation):

```
int imat[] = { 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \
               1, 0, 1, 0, 0, 0, 0, 0, 1, 0, 1, 0, \
               1, 1, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, \
               1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, \
               0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \
               0, 1, 0, 0, 2, 0, 3, 0, 0, 0, 0, 0, \
               0, 1, 0, 1, 0, 0, 0, 0, 0, 1, 0, 1, \
               0, 1, 0, 1, 2, 2, 3, 3, 0, 1, 0, 1, \
               0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, \
               0, 0, 1, 0, 0, 0, 0, 0, 2, 0, 3, 0, \
               0, 0, 1, 1, 0, 1, 0, 1, 0, 0, 0, 0, \
               0, 0, 1, 1, 0, 1, 0, 1, 2, 2, 3, 3  };    (3.4)
```

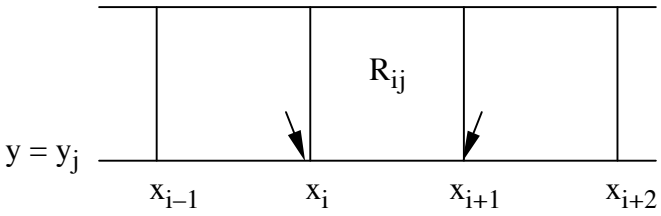
The twelve coefficients in (3.1) are computed by solving a 12×12 linear system, with the above matrix, using Gaussian elimination with partial pivoting. The procedure is to

perform an LU factorization of the matrix exactly once. Then all of the linear systems solves reduce to a much more rapid back-substitution.

The interpolation coefficients are laid out in blocks of 12 in memory, with the coefficients for mesh rectangle $R_{ij}$ starting at location `(j*(nx-1)+i)*12` in the coefficient array.

### *3.2.1. Derivative approximation*

First observe that the four points $(x, f(x,y_j)))$, $x = x_{i-1}, x_i, x_{i+1}, x_{i+2}$ determine a (univariate) cubic in x. One could evaluate the derivative of this cubic at $x_i$ and $x_{i+1}$ to provide estimates of $D_x f_{ij}$ and $D_x f_{i+1,j}$ in (3.2a), and that was done in version 1.1.




A second derivative estimate at $x_i$ can be obtained by using the above procedure with the cubic determined by the four points $(x, f(x,y_j)))$, $x = x_{i-2}, x_{i-1}, x_i, x_{i+1}$. To provide for continuity across mesh boundaries, the average of these two derivative estimates is used to approximate $D_x f_{ij}$. Similarly, the average of the two estimates from $x_{i-1}, x_i, x_{i+1}, x_{i+2}$ and $x_i, x_{i+1}, x_{i+2}, x_{i+3}$ is used to approximate $D_x f_{i+1,j}$. (A similar procedure with the roles of x and y interchanged is used to provide y-derivative estimates.)

Because the necessary neighboring values needed to determine the univariate cubics are not available in the boundary boxes, a non-centered four-point estimate is used to retain cubic precision. This value is set to zero of it is of the opposite sign from the data slope at the boundary.

This is the procedure, implemented in `lip_cubic_derivs`, used all along for the derivative estimates needed for bicubic Hermite coefficients, Section 4.2, below. This averaging process was not carried out for the standard LIP bicubic in version 1.1, and the estimate dropped to quadratic in the normal direction in boundary boxes. Because a different set of four data points was used to estimate $D_x f_{ij}$ in box (i–1,j) and box (i,j), $\partial f/\partial x$ may not even be continuous at $x = x_i$ along the mesh lines. (Similar remarks apply to $\partial f/\partial y$.) At version 1.2, to simplify support of partial setup, it was decided to use the same procedure in both cases, even though this meant that values computed by the standard bicubic differed between the two versions.

In the standard 12-term bicubic case, it turns out that derivatives are still not quite continuous. This is presumably due to the fact that we are not using a complete 16-term bicubic here. Note that the bicubic Hermite interpolant *does* have continuous function and first partial derivatives.

### *3.3. Modification for two-phase data*

A modified version of the bicubic coefficient setup is used for two-phase data, because the standard bicubic behaves very badly at the edges of the two-phase region, where the data suddenly changes from being constant in x (density) to changing very rapidly in this variable. The procedure is to drop to bilinear (a special case of bicubic) inside or at the boundary of the two-phase region.

The two-phase region is detected by the test in `lip_flat_for_2p` (in C notation):

```
if ( (i > 0 && \
     isflat(data[ j   *nx + i-1], data[ j   *nx + i  ])) ||
\
     isflat(data[ j   *nx + i  ], data[ j   *nx + i+1])  ||
\
     (i < nx-2 && \
     isflat(data[ j   *nx + i+1], data[ j   *nx + i+2])) ||
\
     (i > 0 && \
     isflat(data[(j+1)*nx + i-1], data[(j+1)*nx + i  ])) ||
\
     isflat(data[(j+1)*nx + i  ], data[(j+1)*nx + i+1])  ||
\
     (i < nx-2 && \
     isflat(data[(j+1)*nx + i+1], data[(j+1)*nx + i+2])) )
{
   goto Make_it_bilinear;
}                                                              (3.5)
```

Here the logical function `isflat` is defined by

$$\texttt{isflat}(a, b) = ( |a-b| / \max(|a|, |b|) \le \texttt{FLATHRSH} ), \tag{3.6}$$

where the "flatness threshold" `FLATHRSH` is a code parameter that is currently equal to `1.0e-7`. To reduce the amount of extra testing, (3.5) is applied only in boxes $R_{ij}$ which satisfy

$$x_i < 1.5\, x_{crit}, \quad y_j \le 1.1\, y_{crit},$$

where the LEOS access library uses $x_{crit}=\rho_0$, the "normal density" for the material, and $y_{crit}=T_c$, the "critical temperature".

In order to reduce discontinuities between bicubic boxes and neighboring bilinear boxes, the derivative estimates at neighboring points are modified to match the linear slopes.

Note that the above procedure was intended primarily to handle the characteristics of two-phase pressure data. The LEOS access library, however, currently applies this modified cubic setup to all of the two-phase functions: P2p, E2p, and S2p.

### *3.4. Inverse iteration*

Once the appropriate T-interval has been found, as in Section 1.8, we need to solve equation (1.5) for T=T*. The bicubic case is much more complicated than the bilinear case. In this case we have to solve a cubic polynomial equation for y. The present code uses a hybrid secant/bisection algorithm to solve this. Matters are simplified a bit by the fact that, due to the variable transformation (1.3y), we are solving for a root in the interval [0,1].

The iteration tolerance `NEWTON_TOL` is currently set at 1.0e-7. (This was 1.0e-5 in an earlier version, but that was deemed to be insufficient accuracy.) A typical call requires 5–7 iterations, but both smaller and larger values have been observed. (An earlier version that used bisection exclusively required 15 iterations per call.)

### *3.5. The univariate analog*

The cubic functional form on the mesh interval $[x_i, x_{i+1}]$ is:

$$f(x_{int}) = c(x) = a_0 + a_1x + a_2x^2 + a_3x^3, \tag{3.7}$$

where x is as in (2.9).

A univariate cubic function is uniquely determined by the values of the function and its first derivative at two distinct points. The cubic interpolant on the mesh interval $[x_i, x_{i+1}]$ is thus determined by (2.10) and

$$d_k = f'(x_k), \; k = i, i+1. \tag{3.8}$$

Differentiating (3.7) gives

$$f'(x_{int}) = c'(x) = a_1 + 2a_2x + 3a_3x^2 , \tag{3.9}$$

so that we have the four conditions:

$$f_i = f(x_i) = c(0) = a_0; \tag{3.10a}$$

$$d_i = f'(x_i) = c'(0) = a_1; \tag{3.10b}$$

$$f_{i+1} = f(x_{i+1}) = c(x_{i+1}-x_i) = a_0 + a_1(x_{i+1}-x_i) + a_2(x_{i+1}-x_i)^2 + a_3(x_{i+1}-x_i)^3; \tag{3.10c}$$

$$d_{i+1} = f'(x_{i+1}) = c'(x_{i+1}-x_i) = a_1 + 2a_2(x_{i+1}-x_i) + 3a_3(x_{i+1}-x_i)^2. \tag{3.10d}$$

(3.10a) and (3.10b) give us $a_0$ and $a_1$ directly:

$$a_0 = f_i; \tag{3.11a}$$

$$a_1 = d_i. \tag{3.11b}$$

Substituting these into (3.10c) and (3.10d) yields a pair of equations to be solved for the remaining two coefficients. From these we obtain:

$$a_2 = -( 2\Delta_i + \Delta_{i+1} ) ; \tag{3.11c}$$

$$a_3 = ( \Delta_i + \Delta_{i+1} ) / (x_{i+1}-x_i) , \tag{3.11d}$$

where

$$\Delta_k = (d_k - m) / (x_{i+1} - x_i), \quad k = i, i+1 ,$$

and m is the data slope, $m = (f_{i+1} - f_i) / (x_{i+1} - x_i)$ .

If we use the same derivative estimation scheme to produce $d_i$ and $d_{i+1}$ as is used for $D_x f_{mn}$ in the bicubic setup, we obtain a univariate cubic interpolant that is compatible with the bivariate bicubic, in the sense discussed in Section 1.2, above.

As in the bilinear case, the same formulas are used with the obvious change of notation if the independent variable is y instead of x.

# 4. Bicubic Hermite Interpolation (biherm)

This section describes the bicubic Hermite interpolation method (abbreviated "biherm") as currently supported by LIP.

## *4.1. The bicubic Hermite form*

The bicubic Hermite functional form on the mesh rectangle $R_{ij}$ is:

$$\begin{aligned} f(x_{int},y_{int}) \;=\; b(x,y) \;=\; & \\ & a_0\, h_0(x)h_0(y) + a_1\, h_1(x)h_0(y) + a_2\, h_2(x)h_0(y) + a_3\, h_3(x)h_0(y) + \\ & a_4\, h_0(x)h_1(y) + a_5\, h_1(x)h_1(y) + a_6\, h_2(x)h_1(y) + a_7\, h_3(x)h_1(y) + \\ & a_8\, h_0(x)h_2(y) + a_9\, h_1(x)h_2(y) + a_{10} h_2(x)h_2(y) + a_{11} h_3(x)h_2(y) + \\ & a_{12} h_0(x)h_3(y) + a_{13} h_1(x)h_3(y) + a_{14} h_2(x)h_3(y) + a_{15} h_3(x)h_3(y) . \end{aligned} \qquad (4.1)$$

For improved numerical stability, we have performed a change of basis on the bicubic form. Note that this is not equivalent to (3.1), because it contains the full 16 terms required for a general bicubic function. Note also that a bilinear function is *not* a special case.

The (univariate) *cubic Hermite basis functions* that appear in (4.1) are defined by relations:

$$h_0(0) = 1, \quad h_0(1) = 0, \quad h_0'(0) = 0, \quad h_0'(1) = 0; \qquad (4.2a)$$
$$h_1(0) = 0, \quad h_1(1) = 1, \quad h_1'(0) = 0, \quad h_1'(1) = 0; \qquad (4.2b)$$
$$h_2(0) = 0, \quad h_2(1) = 0, \quad h_2'(0) = 1, \quad h_2'(1) = 0; \qquad (4.2c)$$
$$h_3(0) = 0, \quad h_3(1) = 0, \quad h_3'(0) = 0, \quad h_3'(1) = 1. \qquad (4.2d)$$

These lead to the following formulas for the basis functions:

$$h_0(t) \;=\; 1 - 3\,t^2 + 2\,t^3 \;=\; h_1(1-t) \;=\; u^2\,(u + 3\,t) ; \qquad (4.3a)$$
$$h_1(t) \;=\; 3\,t^2 - 2\,t^3 \;=\; t^2\,(t + 3\,u) ; \qquad (4.3b)$$
$$h_2(t) \;=\; t - 2\,t^2 + t^3 \;=\; -h_3(1-t) \;=\; u^2\,t ; \qquad (4.3c)$$
$$h_3(t) \;=\; -\,t^2 + t^3 \;=\; -t^2\,u , \qquad (4.3d)$$

where we have set $u = 1 - t$ .

We note that equation (4.1) can be rewritten in matrix notation:

$$b(x,y) = \mathbf{h}(y)^T \mathbf{A}\, \mathbf{h}(x) , \tag{4.4a}$$

where

$$\mathbf{h}(t) = ( h_0(t), h_1(t), h_2(t), h_3(t) )^T , \tag{4.4b}$$

and

$$\mathbf{A} = \begin{pmatrix} a_0 & a_1 & a_2 & a_3 \\ a_4 & a_5 & a_6 & a_7 \\ a_8 & a_9 & a_{10} & a_{11} \\ a_{12} & a_{13} & a_{14} & a_{15} \end{pmatrix} . \tag{4.4c}$$

For evaluation purposes, formula (4.4a) can be associated either from the left or right, for two possible nested four-element summations. In one case linear combinations of the x-basis functions are formed, and the results are used to form linear combinations of the y-basis functions. The reverse is the case if the other association is chosen. After some experimentation, different associations have been used in the evaluator, depending on the evaluation history, in an attempt to minimize evaluation time. The result is that a biherm evaluation is only 20 to 40 percent slower than a standard bicubic one (depending on whether derivatives are evaluated).

Differentiating (4.4a) with respect to x yields:

$$\partial b(x,y)/\partial x = \mathbf{h}(y)^T \mathbf{A}\, \mathbf{h}'(x) , \tag{4.5}$$

Similarly,

$$\partial b(x,y)/\partial y = \mathbf{h}'(y)^T \mathbf{A}\, \mathbf{h}(x) , \tag{4.6}$$

For bicubic Hermite derivative evaluation, formula (4.5) or (4.6) is used. To provide the necessary values, the Hermite basis derivative evaluator returns $\mathbf{h}'$. The relevant formulas are obtained by differentiating (4.3), namely:

$$h_0'(t) = -6\,t + 6\,t^2 = -h_1'(1-t) = -6tu ; \tag{4.7a}$$
$$h_1'(t) = 6\,t - 6\,t^2 = 6tu ; \tag{4.7b}$$
$$h_3'(t) = 1 - 4\,t + 3\,t^2 = h_4'(1-t) = u\,(u - 2\,t) ; \tag{4.7c}$$
$$h_4'(t) = -2\,t + 3\,t^2 = t\,(t - 2\,u) . \tag{4.7d}$$

### *4.2. Calculating interpolation coefficients*

The bicubic function b(x,y) on mesh box $R_{ij}$, after the transformations (1.3), is uniquely determined by the values of the four quantities

$$b,\ \partial b/\partial x,\ \partial b/\partial y,\ \partial^2 b/\partial x \partial y$$

at the corners of the box. By construction, if the same values of these four quantities are used in adjacent boxes, then these functions are continuous across the box boundaries. This requires using continuous derivative estimates for all partial derivatives that appear here if actual derivative values are unavailable.

A significant advantage of using the Hermite basis is that the interpolation coefficients can be established directly from the interpolation conditions without the need to solve any linear systems. For example, using the relations (4.2) in the functional form (4.1) immediately yields the interpolation conditions (2.2) and the following coefficients:

$$a_0 = b(0,0) = f(x_i,y_j) = f_{ij} ; \quad (4.8a)$$

$$a_1 = b(1,0) = f(x_{i+1},y_j) = f_{i+1,j} ; \quad (4.8b)$$

$$a_4 = b(0,1) = f(x_i,y_{j+1}) = f_{i,j+1} ; \quad (4.8c)$$

$$a_5 = b(1,1) = f(x_{i+1},y_{j+1}) = f_{i+1,j+1} . \quad (4.8d)$$

Note that these four coefficients are in the upper left 4×4 corner of the coefficient matrix A in (4.4c).

Again applying (4.2) to the derivative interpolation conditions (3.2a) shows that the upper right corner of **A** contains the $\partial b/\partial x$–values:

$$a_2 = \partial b(0,0)/\partial x = \Delta x_i \, \partial f(x_i,y_j)/\partial x = \Delta x_i \, D_x f_{ij} ; \quad (4.9a)$$

$$a_3 = \partial b(1,0)/\partial x = \Delta x_i \, \partial f(x_{i+1},y_j)/\partial x = \Delta x_i \, D_x f_{i+1,j} ; \quad (4.9b)$$

$$a_6 = \partial b(0,1)/\partial x = \Delta x_i \, \partial f(x_i,y_{j+1})/\partial x = \Delta x_i \, D_x f_{i,j+1} ; \quad (4.9c)$$

$$a_7 = \partial b(1,1)/\partial x = \Delta x_i \, \partial f(x_{i+1},y_{j+1})/\partial x = \Delta x_i \, D_x f_{i+1,j+1} , \quad (4.9d)$$

where $\Delta x_i = x_{i+1} - x_i$.

Similarly, (3.2b) indicates the lower left corner has the $\partial b/\partial y$–values:

$$a_8 = \partial b(0,0)/\partial y = \Delta y_j \, \partial f(x_i,y_j)/\partial y = \Delta y_j \, D_y f_{ij} ; \quad (4.10a)$$

$$a_9 = \partial b(1,0)/\partial y = \Delta y_j \, \partial f(x_{i+1},y_j)/\partial y = \Delta y_j \, D_y f_{i+1,j} ; \quad (4.10b)$$

$$a_{12} = \partial b(0,1)/\partial y = \Delta y_j \, \partial f(x_i,y_{j+1})/\partial y = \Delta y_j \, D_y f_{i,j+1} ; \quad (4.10c)$$

$$a_{13} = \partial b(1,1)/\partial y = \Delta y_j \, \partial f(x_{i+1},y_{j+1})/\partial y = \Delta y_j \, D_y f_{i+1,j+1} , \quad (4.10d)$$

where $\Delta y_j = y_{j+1} - y_j$.

See Section 3.2.1, above, for a description of the procedure used to provide estimates for the first partial derivatives in (4.9) and (4.10). By using continuous estimates, this assures continuity of first derivatives of the interpolant.

The mixed partial derivatives (or “twists”) fill out the remainder of the coefficient matrix. To see this, differentiate either (4.5) or (4.6) with respect to the other variable to obtain:

$$\partial^2 b(x,y)/\partial x \partial y = \mathbf{h}'(y)^T \, \mathbf{A} \, \mathbf{h}'(x) , \quad (4.11)$$

and the remaining coefficients:

$$a_{10} = \partial^2 b(0,0)/\partial x \partial y = \Delta x_i \, \Delta y_j \, \partial^2 f(x_i,y_j)/\partial x \partial y ; \quad (4.12a)$$

$$a_{11} = \partial^2 b(1,0)/\partial x \partial y = \Delta x_i \, \Delta y_j \, \partial^2 f(x_{i+1},y_j)/\partial x \partial y ; \quad (4.12b)$$

$$a_{14} = \partial^2 b(0,1)/\partial x \partial y = \Delta x_i \, \Delta y_j \, \partial^2 f(x_i,y_{j+1})/\partial x \partial y ; \quad (4.12c)$$

$$a_{15} = \partial^2 b(1,1)/\partial x \partial y = \Delta x_i \, \Delta y_j \, \partial^2 f(x_{i+1},y_{j+1})/\partial x \partial y . \quad (4.12d)$$

Note that the twists could be set to zero without losing the continuity properties, thus reducing the storage requirements to that of the bicubic form, in exchange for a reduction in accuracy. We have not chosen this option for LIP. Instead, the average of the three-point difference formulas in the two coordinate directions applied to the current first derivative estimates is used to estimate the twists in (4.12).

These formulas are used by the biherm setup routine and result in an interpolant that is exact when interpolating data from a biquadratic function. While higher-order twist estimates could be used to obtain complete bicubic precision, it has been decided that it is not worth the extra effort for such a minimal effect on the interpolant.

The interpolation coefficients are laid out in blocks of 16 in memory, with the coefficients for mesh rectangle $R_{ij}$ starting at location `(j*(nx-1)+i)*16` in the coefficient array.

Note that, since bilinear functions are not a subset of bicubic Hermite functions, there is no convenient way to drop to bilinear inside the two-phase region. Consequently, there is no modification of the biherm interpolant for two-phase data comparable to that discussed in Section 3.3. Experience has shown that this interpolant does "ring" near the phase transition boundary, but the behavior is confined to only boxes adjacent to this boundary and is not nearly as pathological as the standard bicubic. To eliminate this "ringing" altogether, use the bimond interpolant, described in the next section.

### *4.3. Monotone bicubic Hermite (bimond)*

Monotonicity preservation is possible with the Hermite form of the bicubic interpolant (see [2]–[4]). We have extended the algorithm described in [4] to handle piecewise monotonic data (such as a typical pressure table) and included it in LIP as the bimond option.

The name "bimond" is historical. The original version of our univariate monotone piecewise cubic interpolation algorithm was implemented in subroutine `MONDER` (`MON`otone `DER`ivatives), a misnomer for the fact that it determined derivative values that resulted in a monotone piecewise cubic Hermite interpolant. We have retained this name for the univariate routine described in Section 4.5, below. Quite naturally, the bivariate version became known as `BIMOND`. The incarnation included in LIP is `BIMOND5` (the fifth release).

In brief outline, the `BIMOND5` algorithm proceeds as follows:

Step 1. Initialize two arrays that characterize the monotonicity properties of the data. (In each segment where the data have a common monotonicity sense, the interpolant will preserve that monotonicity, except perhaps in boxes adjacent to a switch in data monotonicity).

Step 2. Compute initial values for the first partial derivatives $\partial b/\partial x$ and $\partial b/\partial y$ that satisfy a sufficient condition for monotonicity along the mesh lines. This is done by first initializing these values as described above for the biherm option, and

then screening them, possibly reducing derivative magnitudes to satisfy the condition.

Step 3. Construct intervals of acceptable values, containing zero, for the twists $\partial^2 b/\partial x \partial y$. This step may require further reduction in magnitude of first partial derivatives.

Step 4. Compute values for the twists, as described above for the biherm option, and map them into the intervals determined in Step 3.

The primary complication beyond `BIMOND4` [4] occurs in detecting boundaries of monotonicity regions and treating derivative values in adjacent boxes appropriately.

Once the interpolation coefficients have been determined via the `BIMOND5` algorithm, the resulting function is evaluated and/or inverted in exactly the same way as an ordinary biherm interpolant. Only the coefficient setup is different.

The situation becomes rather more complicated in partial setup mode. In mode (2), the `BIMOND5` derivative adjustments can be done once and for all at setup time, so bimond is no different that biherm at evaluation time. The complication comes when only data is available. Depending on the function values, the derivative adjustments may require access to the entire data set. This would require doing the equivalent of a full bimond setup, with its attendant large temporary memory allocation and execution time, to compute coefficients for each new mesh box encountered during the evaluation phase. To reduce the needed storage and time, `lip_evalu_bimond` was modified at version 1.2 to only consider a subset of the data array `nxexp` points in the x-direction and `nyexp` in the y-direction on either side if the current mesh box when computing coefficients. These "expansion parameters" are global variables in `lip_eval2D.c`. The default values are `nxexp`=`nyexp`=3, but the user may reset them by calling `lip_set_bimond_exp` prior to calling `lip_evalu_bivar`. The larger these parameters are, the more temporary storage and execution time is required, but the more likely the results will agree with those from full coefficient setup mode.

### *4.4. Inverse iteration*

The bicubic Hermite case is handled much like the standard bicubic case, discussed in Section 3.4, above. The same iteration procedure is used. The only difference is that the cubic being solved is represented in Hermite form, rather than power form.

Because of the above complication, the current version of LIP does not support inversion of a bimond interpolant in partial setup mode, except by use of `lip_inv_general`.

### *4.5. The univariate analog*

The cubic Hermite functional form on the mesh interval $[x_i, x_{i+1}]$ is:

$$f(x_{int}) = c(x) = a_0\, h_0(x) + a_1\, h_1(x) + a_2\, h_2(x) + a_3\, h_3(x), \qquad (4.13)$$

where x is as in (1.3x), and the $h_k(x)$ are as in (4.3). (We *do* divide by the interval length here, because the $h_k$ are defined on the unit interval [0,1].)

Differentiating (4.13) and using the defining characteristics of the cubic Hermite basis functions (4.2) yields the four formulas:

$$a_0 = c(0) = f(x_i) = f_i \; ; \tag{4.14a}$$

$$a_1 = c'(0) = \Delta x_i \, f'(x_i) = \Delta x_i \, d_i \; ; \tag{4.14b}$$

$$a_2 = c(1) = f(x_{i+1}) = f_{i+1} \; ; \tag{4.14c}$$

$$a_3 = c'(1) = \Delta x_i \, f'(x_{i+1}) = \Delta x_i \, d_{i+1} \; , \tag{4.14d}$$

These immediately give us the fact that the cubic Hermite function (4.13) satisfies the conditions (2.10) and (3.8) that are necessary and sufficient to uniquely define a cubic function on $[x_i, x_{i+1}]$.

If we use the same derivative estimation scheme to produce $d_i$ and $d_{i+1}$ as is used for $D_x f_{mn}$ in the bicubic Hermite setup, then we obtain a univariate cubic Hermite interpolant that is compatible with its bivariate counterpart, in the sense discussed in Section 1.2, above.

In order to provide a univariate interpolant (monder) that is compatible with bimond, we have included an algorithm that uses essentially the procedure of Step 2 of `BIMOND5` (see Section 4.3, above) to compute a piecewise monotonic cubic Hermite interpolant. Strictly speaking, monder will be compatible with the bimond interpolant only of no Step 3 first derivative modifications were required along the lowest isotherm.

# 5. Piecewise Biquadratic Interpolation

This section describes the biquadratic interpolation method as currently supported by LIP. This form was inherited from the LEOS interpolation package.

### *5.1. The biquadratic form*

The biquadratic form is *not* recommended as a general bivariate interpolator. It is included in LIP only as a means to provide an interpolant for the old EOP data that emulates that provided in EOS4 [5]. (This is a concession to allow the LEOS access library to load with LIP instead of using the original LEOS interpolants.) There is no transformation to the normalized variables (x,y) in this case; that is, $(x,y) = (x_{int},y_{int})$ here. This is to be as close to the EOS4 interpolant as possible (outside of language and computer arithmetic differences).

The biquadratic functional form on the mesh rectangle $R_{ij}$ is:

$$f(x_{int},y_{int}) = q(x,y) = a_0 + a_1x + a_2y + a_3x^2 + a_4y^2 + a_5xy + a_6x^2y + a_7xy^2 + a_8x^2y^2. \tag{5.1}$$

NOTE: This form is not fully supported; in particular, there is no univariate equivalent.

### 5.2. Calculating interpolation coefficients

For compatibility with the past, the coefficient calculation algorithm used is a C translation of the one in EOS4 [5]. (Further details will not be given here.)

The interpolation coefficients are laid out in blocks of nine in memory, with the coefficients for mesh rectangle $R_{ij}$ starting at location `(i*(nx-1)+j)*9` in the coefficient array.

### 5.3. Inverse iteration

The biquadratic case is intermediate in complication between bilinear and bicubic. In this case, a quadratic equation has to be solved, once we determine the interval $[T_i,T_{i+1}]$ containing the target T*. For compatibility with the past, the algorithm used is a C translation of the one in EOS4 [5], with some of the special case coding omitted.

# 6. Piecewise Birational Interpolation

This section describes the birational interpolation method, which was added to LIP at version 1.3.

### 6.1. The birational form

The birational form does not fit naturally into the standard LIP formulation. According to the available LANL documentation [7], the univariate rational form is the ratio of a cubic and a linear polynomial:

$$r(t) = [f_k + A_k (t - t_k) + B_k (t - t_k)^2 + D_k (t - t_k)^3 ] \ / \ [1+ C_k (t - t_k)], \qquad (6.1)$$

for t in the k-th mesh interval, $[t_k, t_{k+1}]$. The coefficients that appear in (6.1) are not computed explicitly, but rather the function value is developed from the data values in the course of evaluation.

The birational form is obtained, in principle, by applying this procedure in each of the mesh directions. It is not guaranteed that the univariate rational interpolator is compatible in the sense of Section 1.2.

### 6.2. Evaluation

The code provided in LIP was created by adapting C code developed at LANL to LIP specifications. As noted in Section 7.8, below, this is contained in files `lip_BiRatInterp.c` and `lip_RatInterp.c`.

# 7. Software Organization

LIP is written in ANSI standard C for portability, but an object-oriented design is emulated in the code. The LIP source code is described in this section. First comes an overview illustrating how to use the software. An outline of the source code organization follows this. Then come detailed descriptions of the source files, grouped by function.

# 7. Software Organization

## *7.1. Overview*

To use LIP to interpolate in a given data table, one must first create a LIP interpolation object, populate it with the data, and create a coefficient array for the desired interpolation method. Then one can pass this object to other functions to do desired forward or inverse interpolations.

A summary of this process follows, with illustrative examples. For a more complete example of package usage, refer to Section 8, below.

Those of you familiar with LIP version 1.0 will know that the process originally required several steps, each involving a call to one of the LIP functions:

(1) Create a LIP interpolation object (macro `FMAKE`).
(2) Initialize the object (function `lip_init_interp`).
(3) Add the data to it (function `lip_add_data`).
(4) Compute interpolation coefficients of the chosen interpolation type (function `lip_calc_coeff`).

A major change in version 1.1 was the introduction of a function `lip_setup_interp` that combines these steps into a single call. From the user's point of view, this reduces the amount of coding required to get started. Note that the object must now appear as a pointer to a pointer in the `lip_setup_interp` call.

New step (1) Create and populate an interpolation object with interpolation coefficients of the chosen interpolation type. (The following example uses pressure as a function of density and temperature, but it could be any two-dimensional data set. It uses bicubic Hermite interpolation.)

```
#include "LIP_proto.h"  /* LIP function prototypes. */
   ...
LIP_interp *interp ;
LIP_meth int_type=LIP_HERM ;
Integer job_flag, retval ;

job_flag = 3 ;   /* Do full coefficient setup. */

retval = lip_setup_interp ( &interp, "rho", ndens, dens,
                            "T", ntemp, temp, "P", pval,
                            int_type, job_flag );
```

New step (2) Pass `interp` on to functions that will do evaluations and/or inversions using it. (The following will interpolate at `npts` points, with the results in `fint`. Flag `extr_flag` has been set to select linear extrapolation, as discussed in Section 1.7. Only function values have been requested, so `dfdx` and `dfdy` will not be referenced.)

```
Integer extr_flag=1;
Logical calcf=TRUE, calcdfdx=FALSE, calcdfdy=FALSE;
```

```
retval = lip_evalu_bivar( interp, int_type, extr_flag,
                          xint, yint, npts, calcf, fint
                          calcdfdx, dfdx, calcdfdy, dfdy );
```

New step(3) When through using this object, free up space that has been allocated for it. *Note* ***incompatibility*** *with version 1.0*: While the old four-step process can still be used to set up the object, if desired, the `lip_free_interp` call sequence has changed, so the object must now appear as a pointer to a pointer. (Note that `lip_free_interp` now de-allocates the object, so an `SFREE` is not needed.)

```
retval = lip_free_interp( &interp );
```

The user who is interested in the reduced storage requirements made available via the partial setup options discussed in Section 1.4, above, should refer to Section 7.3, below.

### *7.2. LIP data types and memory management*

In the above we referred to `FMAKE` and `SFREE`, which are memory management macros defined in `LIP_macros.h`. These were written to emulate the PACT [6] memory management facility, which was used in the original version of the LEOS access library. Their call sequences are:

`FMAKE`: Allocate space for a single object of type `type`.

```
obj = FMAKE( type, string );
```

Here `obj` is a pointer to the created object and `string` is an identifier, typically of the form `"FNAME:obj"`, where `FNAME` is the name of the function issuing this call.

`FMAKE_N`: Allocate space for an array of `n` objects of type `type`.

```
obj = FMAKE_N( type, n, string );
```

Here `obj` is a pointer to the created array and `string` is an identifier, typically of the form `"FNAME:obj"`, where `FNAME` is the name of the function issuing this call. (See the sample program for examples.)

`SFREE`: De-allocate space for an object previously allocated by `FMAKE` or `FMAKE_N`:

```
SFREE( obj );
```

`LIP_macros.h` also contains definitions for `min`, `max`, and other useful macros.

All of the LIP source files also include `LIP_Ftype.h`, which defines Fortran-compatible data types such as `Integer`, `Real8`, `Logical` used above. Because header files `LIP_Ftype.h` and `LIP_macros.h` are included in `LIP_proto.h`, there is no need for the user to explicitly include them.

### *7.3. Partial Setup Options*

In order to provide ready access to the full range of setup options now available in LIP, we give below the complete user interface for `lip_setup_interp`. (This was taken from the source code and edited to better fit the page format.) Refer to Appendix A for definitions of the `int_type` and `setup_type` values mentioned here.

```
Integer lip_setup_interp(      LIP_interp **interp,
                         const char *xname,
                         const Integer nx,
                         const Real8 *x,
                         const char *yname,
                         const Integer ny,
                         const Real8 *y,
                         const char *fname,
                         const Real8 *f,
                         const LIP_meth int_type,
                         const Integer job_flag )

/*************************************************************
*************************************************************
This function initializes and populates a LIP interpolation
object.  Partial setup options are provided, as well as the
standard full coefficient array calculation.

Arguments:
   interp is a pointer to a newly created LIP_interp
          object.  Because its memory space is allocated
          within this function, this is a pointer to a
          pointer.  Thus the ADDRESS of the declared object
          should appear in the call list.  Example:
            LIP_interp *my_interp;
            retval = lip_setup_interp( &my_interp, xname,
                                       ...);
            < Code that passes my_interp to an evaluator,
              inverter, etc. >
          The allocated space will be freed by a call to
          lip_free_interp.
   xname  is the name to be associated with the x-values.
   nx     is the number of x-values.
   x      is a pointer to the array of x-values to be
          added.
   yname  is the name to be associated with the y-values.
   ny     is the number of y-values.
   y      is a pointer to the array of y-values to be
          added.
   fname  is the name to be associated with the f-values.
   f      is a pointer to the array of f-values to be
          added.
```

```
   int_type is the interpolation type for this object.
          When job_flag<3, an input value of 0 will be
          interpreted as "I don't want to set it yet,"
          which means it will have value LIP_INVALID on
          return.  This can be overridden by a subsequent
          lip_set_int_type call or by the int_type argument
          to lip_evalu_univar or lip_evalu_bivar.
   job_flag indicates the type of setup to be performed.
          job_flag = 0 : only add the data to interp.
                   On successful completion, setup_type
                   will be LSU_DATA.
          job_flag = 1 : approximate first partial
                   derivatives, using a method consistent
                   with int_type.  (Not applicable if
                   int_type = LIP_LIN or LIP_RAT.  Acts
                   like job_flag=0 in this case.)  On
                   successful completion, setup_type will
                   be LSU_1DER or LSU_2DER, depending on
                   whether 1-D or 2-D data was provided.
          job_flag = 2 : approximate first partial
                   derivatives and twists, using a method
                   consistent with int_type.  (Only
                   applicable for 2-D data with int_type =
                   LIP_HERM or LIP_MONO.  As above, acts
                   like job_flag=0 if int_type = LIP_LIN or
                   LIP_RAT.)  On successful completion,
                   setup_type will be LSU_3DER.
         job_flag = 3 : compute full coefficient array for
                   int_type interpolation.  (Not applicable
                   if int_type = LIP_RAT.)  On successful
                   completion, setup_type will be LSU_COEF.

  Note: If nx=0, x may be NULL and is not checked or added.
        If ny=0, y may be NULL and is not checked or added.
        (These are 1-D data sets.)

Input arguments:  xname, nx, x, yname, ny, y, fname, fval,
                  int_type, job_flag.

Output arguments: interp.

Return value:  The return value, retval, should be zero.
  A positive return value is a warning, indicating that
```

```
retval of the array fields in interp were non-NULL, so
were freed before allocation.  (This probably indicates
that lip_setup_interp was called with a previously
populated interp.)
The possible fatal error returns are:
  retval = -1800 : trouble creating interp.
  retval = -1801 : illegal value of job_flag.
  retval = -1802 : illegal or unsupported value of
                   int_type.
  retval = -1805 : too few data points for cubic
                   interpolation.
  retval = -1810 : trouble creating temporary workspace.
  retval = -1820 : error return from lip_monomod1D.
  retval = -1821 : error return from PBHpm.
  This version may also return retval from a called
  function.
```

### *7.4. Source code organization*

The LIP source tree has the following organization. Directories are in **boldface** type.

**lip**
- COPYRIGHT
- INSTALL
- LIP_Ftype.h
- Makefile.in
- README
- RELEASE_NOTICE
- TESTING
- **aux_source**
- **config**
- configure
- **data**
- **docs**
- **source**
- **test**
- **utility**

The contents of these files/directories are as follows:

`COPYRIGHT` : standard copyright notice.

`INSTALL` : instructions for building `liblip.a` and the test and utility codes.

`LIP_Ftype.h` : header file for defining Fortran compatible data types. This is here, rather than in **`source`**, because it is used by the `configure` script as a check for being in the top-level source code directory.

`Makefile.in` : This is a template for the top level `Makefile` for the package, that will be generated when `configure` is run. Read `INSTALL` first.

`README` : contains information on the contents of this top-level directory.

`RELEASE_NOTICE` : notice of the current version of LIP and how it differs from the previous version(s).

`TESTING` : instructions for running the test codes and interpreting the results.

**`aux_source`** : contains auxiliary functions and codes used by one or more of the LIP test or utility codes.

**`config`** : contains all scripts and files for configuring LIP.

`configure` : script for configuring the build process. Read `INSTALL`.

**`data`** : contains various data sets used for testing parts of LIP.

**`docs`** : contains LIP documentation files, as well as tools for creating `user_docs` files from LIP source files.

**`source`** : contains the actual source code for LIP. The contents of this directory will be discussed in the following sections.

**`test`** : contains various programs for testing parts of LIP. The individual test codes are in separate subdirectories, each with its own `README` file.

**`utility`** : contains various LIP utility programs and procedures for building and testing them. The individual utility codes are in separate subdirectories, each with its own `README` file.

### *7.5. LIP data structures and setup functions*

The following files deal with defining, initializing, populating, and interrogating LIP interpolation objects. Refer to `lip/docs/user_docs_setup` for the user interfaces for the setup functions and `lip/docs/user_docs_getters` for the user interfaces for the interrogation functions.

`lip_setup.c` : functions to initialize, populate, and free a LIP interpolation object.

`LIP_setup.h` : definition of the `LIP_interp` data type, which sets up a LIP interpolation object, and prototypes for the LIP setup functions.

`lip_setup_interp.c` : comprehensive function to initialize and populate a LIP interpolation object. This uses several functions from `lip_setup.c`. It is in a separate file and its prototype is in `LIP_proto.h`, because it calls functions

from several other source files whose prototypes are declared there. (See Section 7.3, above, for more details on this function.)

`lip_utility.c` : functions to interrogate the contents of a LIP interpolation object.

`LIP_utility.h` : prototypes for the functions in `lip_utility.c`. (Of course, this `#include`'s `LIP_setup.h`.)

Routines included in file `lip_setup.c` are:

`lip_init_interp()` : initialize an interpolation object.

`lip_valid_setup()` : validate the object's `setup-type`.

`lip_add_data()` : add data to an interpolation object.

`lip_add_1der()` : add one derivative (for 1-D data) to an interpolation object.

`lip_add_2der()` : add two derivatives (for 2-D data) to an interpolation object.

`lip_add_twists()` : add twists (for 2-D data) to an interpolation object.

`lip_get_nbasfcns()` : get value of `nbasfcns` (called `ncoef` in the table in Section 1.3) for provided `int_type`. (N.B.: this function is also used to check for a valid `int_type` value.)

`lip_add_coeff()` : add full coefficient array (calculated elsewhere) to an interpolation object.

`lip_free_interp()` : free space for all array fields, then de-allocate the object.

Routines included in file `lip_utility.c` are:

The following functions return specified fields from a `LIP_interp` object:

`lip_get_setup_type()` : get the `setup_type` value from an interpolation object. (See Appendix A for allowable values.)

`lip_get_xname()` : get the `xname` (name associated with the first independent variable) from an interpolation object.

`lip_get_nx()` : get the `nx`-value from an interpolation object.

`lip_get_x()` : get the `x` array from an interpolation object.

`lip_get_yname()` : get the `yname` (name associated with the second independent variable) from an interpolation object.

`lip_get_ny()` : get the `ny`-value from an interpolation object.

`lip_get_y()` : get the `y` array from an interpolation object.

`lip_get_fname()` : get the `fname` (name associated with the dependent variable) from an interpolation object.

`lip_get_fval()` : get the `fval` (function value) array from an interpolation object.

`lip_get_dfdx()` : get the `dfdx` array from an interpolation object.

`lip_get_dfdy()` : get the `dfdy` array from an interpolation object.

`lip_get_twists()` : get the `twists` array from an interpolation object.

`lip_get_coeff()` : get the `coeff` array from an interpolation object.

`lip_get_int_type()` : get the `int_type` value from an interpolation object. (See Appendix A for allowable values.)

*Caution*: In the case of an array field, the return value from the associated function is a pointer, not a copy of the array.

Other utility functions:

`lip_print_interp()` : print the contents of an interpolation object in a readable format.

### *7.6. LIP general utility functions*

The following files contain various general utilities for LIP.

`lip_int_util.c` : miscellaneous utility functions used by one or more of the LIP evaluators or coefficient generators.

`LIP_int_util.h` : prototypes for the LIP interpolation utilities contained in file `lip_int_util.c`.

`lip_vers_date.c` : functions to return the version number and date for the current LIP package. (This `#include`'s `LIP_config.h`, which is created by the LIP build process.) Prototypes for these functions are in `LIP_int_util.h`.

`lip_error.c` : defines the LIP error handling functions.

`LIP_error.h` : prototypes for the functions in `lip_error.c`. (This is `#included` in `LIP_setup.h` and `LIP_int_util.h`.)

Routines included in file `lip_int_util.c` are:

`lip_dcopy()` : copy the contents of a `Real8` array to another.

`lip_dswap()` : swap the contents of two `Real8` arrays.

`lip_fun3c()` : three-point difference derivative approximation.

`lip_p3d()` : compute the derivative of the cubic polynomial that interpolates a given set of data points.

`lip_cubic_derivs()` : compute derivative estimates suitable for piecewise cubic interpolation in a given (x,y) data table. (See Section 3.2.1.)

`lip_cubic_der2_cell()` : a modification of `lip_cubic_derivs` that computes only two derivative estimates and requires only 6 input f-values.

`lip_cubic_est()` : compute "standard" derivative estimate for `lip_cubic_derivs`.

`lip_cubic_est2()` : a modification of `lip_cubic_est` that only requires five f-values, not a whole slice.

`lip_twist_est()` : estimate the "twist" at a point from independent variable arrays and user-supplied first derivative arrays.

`lip_twist_est_box()` : a box-oriented version of `lip_twist_est` that uses only local derivative values.

`lip_deriv_est_box()` : compute derivative estimates needed by `lip_twist_est_box`.

`lip_hbasisf()` : evaluate the four Hermite basis functions at a point in [0,1].

`lip_hbasisd()` : evaluate derivatives of the four Hermite basis functions at a point in [0,1].

`lip_mach()` : emulate SLATEC floating point properties function.

`lip_fsign()` : emulate Fortran's SIGN function.

`lip_sign_test()` : emulate the PCHIP sign-testing function.

`lip_lookup()` : LIP table look-up routine. (See Section 1.5.)

Routines included in file `lip_vers_date.c` are:

`lip_package_version()` : return the interpolation package version number.

`lip_package_date()` : return the interpolation package date.

Routines included in file `lip_error.c` are:

`lip_error_print()` : print an error message to the LIP global error message string `lip_errmsg`.

### *7.7. LIP coefficient generation*

The following files contain functions for computing interpolation coefficients for a LIP interpolation object. Refer to `lip/docs/user_docs_interp` for the user interfaces for the coefficient generation and interpolation functions. See Appendix A for a list of supported interpolation types.

`LIP_proto.h` : prototypes for the LIP coefficient generation and interpolation functions. (This contains `#include`'s for `LIP_setup.h`, `LIP_utility.h`, and `LIP_int_util.h`, so that a user code need only include `LIP_proto.h`.)

`lip_coeff.c` : functions to calculate interpolation coefficients for a LIP interpolation object.

`lip_setup_bimond.c` : separate code for "bimond", the `LIP_MONO` coefficient setup (two-dimensional case).

`pbhpm.c` : functions that do the actual work for `lip_setup_bimond`. The primary function is PBHpm (Piecewise Bicubic Hermite interpolation that preserves monotonicity).

`LIP_PBH.h` : prototypes for the PBH functions in `pbhpm.c`.

`pchsubs.c` : two functions from the old PCHIC package used by the PBH functions.

`LIP_PCH.h` : prototypes for the functions in `pchsubs.c`.

Routines included in file `lip_coeff.c` are:

`lip_set_critvals()` : set critical values for `LIP_CUBM`.

`lip_get_critvals()` : retrieve critical values for `LIP_CUBM`. (Used by `lip_calc_coeff`.)

`lip_calc_coeff()` : compute a coefficient array and add it to an existing LIP interpolation object. This is the primary user-callable function in this file. (If `int_type`= `LIP_CUBM`, it is necessary to call `lip_set_critvals` first.)

`lip_setup_linear()` : calculate linear interpolation coefficients.

`lip_setup_cubic()` : calculate cubic interpolation coefficients.

`lip_setup_hermit()` : calculate cubic Hermite interpolation coefficients.

`lip_setup_monder()` : calculate piecewise monotonic cubic Hermite interpolation coefficients.

`lip_monomod1D()` : used by `lip_setup_monder` to modify derivatives to be suitable for piecewise monotonicity.

`lip_1D_end_mods()` : post-process previously setup 1-D cubic to enforce user-specified boundary derivatives.

`lip_setup_bilinear()` : calculate bilinear interpolation coefficients (`LIP_LIN`).

`lip_setup_bicubic()` : calculate interpolation coefficients for the 12-term bicubic form (`LIP_CUB`).

`lip_bicubic_matrix()` : set up and factor the `lip_setup_bicubic` system matrix.

`lip_bicubic_rhs()` : compute the right-hand-side vector for the `lip_setup_bicubic` linear system.

`lip_factor()` : compute the LU factorization of a matrix. (Used by `lip_bicubic_matrix`.)

`lip_solve()` : solve a linear system, given its LU factorization. (Used by `lip_setup_bicubic`.)

`lip_setup_bicubic2p()` : calculate bicubic interpolation coefficients for two-phase data (`LIP_CUBM`). (A modification of `lip_setup_bicubic`.)

`lip_flat_for_2p()` : function used by `lip_setup_bicubic2p` to detect two-phase data.

`lip_setup_biherm()` : calculate bicubic Hermite interpolation coefficients (`LIP_HERM`).

`lip_bicubic_derivs()` : calculate derivative estimates suitable for bicubic Hermite interpolation (`int_type=LIP_HERM` or `LIP_MONO`)

`lip_coeff_biherm()` : perform the actual coefficient calculations after `lip_setup_biherm` estimates first derivatives. (Also used by `lip_setup_bimond`.)

`lip_coeff_bh_one()` : set up the bicubic hermite interpolation coefficients for one mesh box. (Used by `lip_coeff_biherm`.)

`lip_setup_biquad()` : calculate biquadratic interpolation coefficients (`LIP_QUAD`).

Routines included in file `lip_setup_bimond.c` are:

`lip_setup_bimond()` : calculate monotone bicubic Hermite interpolation coefficients (`LIP_MONO`). (This is basically an interface routine for `PBHpm`, described below.)

File `pbhpm.c` contains the C version of the Fortran function `PBHPM`, along with all of its subsidiary routines. Routines included are:

`PBHpm` : main control routine for BIMOND5 coefficient setup.

The names for its subsidiary routines were inherited from the Fortran version.

`pbhinit_` : PBHCOM Initialization Routine.

`pbhm1a_` : Step 1 of bicubic Hermite derivative algorithm.

`pbhcz_` : BIMOND Compress Zero string routine.

`pbhm2b_` : Step 2 of bicubic Hermite derivative algorithm.

`pbhm3a_` : Step 3 of bicubic Hermite derivative algorithm.

`pbhxmb_` : Piecewise Bicubic Hermite X-Monotonicity checker.

`pbhymb_` : Piecewise Bicubic Hermite Y-Monotonicity checker.

`pbhsda_` : BIMOND String Decomposition Routine.

`pbhsg_` : Piecewise Bicubic Hermite SiGn routine.

`pbhtpa_` : BIMOND Transition element Processor.

`pbhts_` : Modified BIMOND Two-sweep Algorithm.

`pbhm4a_` : Step 4 of bicubic Hermite derivative algorithm.

`pbhtw_` : Piecewise Bicubic Hermite TWist routine.

`adc3p_` : Approximate Derivative by Centered 3-Point formula.

File `pchsubs.c` contains the C versions of needed functions from the Fortran package `PCHIP`. Routines included are:

`pchcs8_` : `PCHIC8` Monotonicity Switch Derivative Setter. (Used by `PBHpm` to adjust initially estimated derivatives.)

`pchsw8_` : `PCHCS8` Switch Excursion Limiter. (Used by `pchcs8_`.)

### *7.8. LIP interpolation functions*

The following files contain functions for forward and inverse interpolation using a LIP interpolation object. Refer to `lip/docs/user_docs_interp` for the user interfaces for the coefficient generation and interpolation functions. See Appendix A for a list of supported interpolation types.

`LIP_proto.h` : prototypes for the LIP coefficient generation and interpolation functions. (This contains `#include`'s for `LIP_setup.h`, `LIP_utility.h`, and `LIP_int_util.h`, so that a user code need only include `LIP_proto.h`.)

`lip_BiRatInterp.c` : separate code for birational interpolation.

`lip_RatInterp.c` : separate code for (univariate) rational interpolation.

`lip_eval1D.c` : LIP one-dimensional evaluation functions.

`lip_eval2D.c` : LIP two-dimensional evaluation functions.

`lip_inverse.c` : functions for inverting two-dimensional interpolants. (Currently the package only supports inversion in the second independent variable.)

Routines included in file `lip_eval1D.c` are:

`lip_evalu_univar()` : general univariate interpolant evaluator. (This is the user-callable function for 1-D interpolation.)

`lip_evalu_cell()` : univariate interpolant evaluator with known cell indices.

The following four functions are called by `lip_evalu_cell`:

`lip_evalu_linear()` : used when `int_type=LIP_LIN`.

`lip_evalu_cubic()` : used when `int_type=LIP_CUB` or `LIP_CUBM`.

`lip_evalu_hermit()` : used when `int_type=LIP_HERM` or `LIP_MONO`.

`lip_evalu_rat()` : used when `int_type=LIP_RAT`.

(Note that `lip_evalu_rat` and its evaluator `lip_RatInt` are in separate file `lip_RatInterp.c`.)

The following auxiliary function is also in this file:

`lip_cells()` : process an index array for `lip_evalu_univar`.

Routines included in file `lip_eval2D.c` are:

`lip_set_bimond_exp()` : set the mesh expansion parameters for `lip_evalu_bimond`. (See end of Section 4.3.)

`lip_get_bimond_exp()` : get the mesh expansion parameters to be used by `lip_evalu_bimond`.

`lip_evalu_bivar()` : general bivariate interpolant evaluator. (This is the user-callable function for 2-D interpolation.)

`lip_evalu_box()` : bivariate interpolant evaluator with known box indices.

The following seven functions are called by `lip_evalu_box`:

`lip_evalu_bilinear()` : used when `int_type=LIP_LIN`.

`lip_evalu_bicubic()` : used when `int_type=LIP_CUB`.

`lip_evalu_bicubic2p()` : used when `int_type=LIP_CUBM`.

`lip_evalu_biherm()` : used when `int_type=LIP_HERM`.

`lip_evalu_bimond()` : used when `int_type=LIP_MONO`.

`lip_evalu_biquad()` : used when `int_type=LIP_QUAD`.

`lip_evalu_birat()` : used when `int_type=LIP_RAT`.

(Note that `lip_evalu_birat` and its evaluator `lip_BiRatInt` are in separate file `lip_BiRatInterp.c`.)

The following auxiliary functions are also in this file:

`lip_boxes()` : process a pair of index arrays for `lip_evalu_bivar`.

`lip_coeff_bh_one2()` : a modified version of `lip_coeff_bh_one` for use only by evaluators.

`lip_evalu_bihermite()` : does the evaluations for `lip_evalu_biherm` and `lip_evalu_bimond`.

Routines included in file `lip_inverse.c` are:

`lip_inverse_vals()` : general inverter. (This is the user-callable function for inverse interpolation.)

`lip_inv_coeff()` : used when full coefficient setup has been done.

`lip_inv_bilinear()` : used by `lip_inv_coeff` when `int_type= LIP_LIN`.

`lip_inv_biquad()` : used by `lip_inv_coeff` when `int_type= LIP_QUAD`.

`lip_in_intrv()` :used by `lip_inv_biquad` to check whether a point is in a specified interval.

`lip_inv_bicubic()` : used by `lip_inv_coeff` when `int_type= LIP_CUB` or `LIP_CUBM`.

`lip_inv_biherm()` : used by `lip_inv_coeff` when `int_type= LIP_HERM` or `LIP_MONO`.

`lip_inv_partial()` : used for partial coefficient setup case.

`lip_inv_bilin()` : used by `lip_inv_partial` when `int_type= LIP_LIN`.

`lip_inv_bicub()` : used by `lip_inv_partial` when `int_type= LIP_CUB`.

`lip_coef_box_bicub()` : used by `lip_inv_bicub` to compute local interpolation coefficients as needed.

`lip_solve_bicub()` : used by both `lip_inv_bicubic` and `lip_inv_bicub` to solve the univariate cubic equation that determines a particular bicubic inverse value.

`lip_inv_biher()` : used by `lip_inv_partial` when `int_type= LIP_HERM`.

`lip_coef_box_biher()` : used by `lip_inv_biher` to compute local interpolation coefficients as needed.

`lip_solve_biher()` : used by both `lip_inv_biherm` and `lip_inv_biher` to solve the univariate cubic equation that determines a particular bicubic Hermite inverse value.

`lip_inv_general()` : general `int_type`-independent inverter.

# 8. An Example of Package Usage

This section contains a complete program that illustrates the use of LIP to solve an interpolation problem. It first reads a set of sample data using function `readeos` (see Appendix C). It then sets up two LIP interpolation objects for this data, one using bicubic Hermite interpolation (`int_type=LIP_HERM`), the other using BIMOND (`int_type =LIP_MONO`). It first evaluates these interpolants on the input data mesh and checks the interpolation accuracy and signs of derivatives at the mesh points. Then it evaluates each at a selection of points in the interior of a mesh box. For the provided data (see Appendix D), mesh box (4,0) is known to give interpolation procedures trouble, so several interior points in that box are selected to study the behavior of the two interpolants there. The test results are given in Appendix E.

Note: To improve the readability of the example code, optional debug printouts and lines that test returned values from LIP functions have been omitted here. They are included in the available source code, which is in `lip/test/sample`.

```
/************************************************
*                                               *
*    Sample code illustrating the use of LIP    *
*                                               *
************************************************/

#include <math.h>
#include <float.h>
#include <stdlib.h>
#include <stdio.h>

/* The following is for the LIP test build procedure. */
#ifdef HAVE_CONFIG_H
#include "LIP_config.h"
#endif

#include "LIP_macros.h"  /* For various macro definitions. */
#include "LIP_proto.h"   /* LIP function prototypes. */

/* Define maxabs function (min and max defined in LIP_macros.h). */
#define maxabs(A,B) ( max( fabs(A), fabs(B) ) )

/* Tolerance for relative error tests. */
#define ERRTOL 1.0e-14

char errmsg[2*MAXLINE];  /* Test global error message string (2 lines). */
char lip_errmsg[MAXLINE];  /* LIP global error message string. */

/* Prototype for data read function. */
Integer readeos(const char *filename,
                Integer *nx, Real8 **x, Integer *ny, Real8 **y,
                Real8 **f, char *fname);
```

```
/**********************/
/* Start of main code */
/**********************/

int main()

/*************************************************************************
*
*************************************************************************
*
* This sample code defines both a BIHERM and BIMOND interpolant to an
* input data set.  It first evaluates both on the input mesh and
* verifies that both reproduce the data within machine precision.
* It then shows that the BIHERM interpolant is not monotonic, but the
* BIMOND one is.
*
* Because EOS (equation of state) data is used for this example,
* variable names rho and t are used instead of x and y.
*
* Change record:
* (yymmdd means 20yy/mm/dd)
*  080814  Initial implementation by Fred N. Fritsch, LEOS Development
*          Team.
*  081118  Modified to use new lip_setup_interp. (FNF)
*
*************************************************************************
*
*************************************************************************
/

/* Implementation Note:                                                 */
/*   Function values computed by BIHERM are denoted by p1val and the */
/*   associated derivatives by dp1dr, dp1dt.                            */
/*   Function values computed by BIMOND are denoted by p2val and the */
/*   associated derivatives by dp2dr, dp2dt.                            */

{

 /* Declare data variables. */
    char filename[80];  /* Name of input file. */
    Integer nrho, nt;
    Real8   *f, *rho, *t;
    char fname[8];

 /* Declare two LIP interpolation objects. */
    LIP_interp *interp_herm;  /* For the BIHERM interpolant. */
    LIP_interp *interp_mono;  /* For the BIMOND interpolant. */
    LIP_meth int_type;
    Integer job_flag, retfree;

 /* Declare interpolation variables. */
    Integer extr_flag=0;  /* Set for constant extrapolation. */
    Integer npts;
    Logical calcf, calcdr, calcdt;
    Real8   *rhoval, *tval;
    Real8   *dp1dr, *dp1dt, *p1val;
    Real8   *dp2dr, *dp2dt, *p2val;
```

```
 /* Declare other variables. */
    Integer i, j, k, retval;
    Integer nbad1, nbad2;
    Real8   drho, dt, error, rhosave;


/* Begin executable statements */
/* =========================== */

    printf ("\n\t LIP sample code");
    printf ("\n\t-----------------\n");

    /* Get name of input file and read data from it. */

    printf("\n Type file name.\n");
    if ( scanf("%s", filename) != 1) {
        printf("\n*** Trouble reading filename.\n\n");
        printf("     Aborting run.\n");
        return -999;
    }
    printf("\n");   /* Skip a line before any readeos output. */

    retval = readeos(filename, &nrho, &rho, &nt, &t, &f, fname);
    /* Note: on successful return, readeos will have allocated space */
    /*       for arrays rho, t, f.                                   */

    /* Should check value of retval and take appropriate action. */

    printf("\n readeos returned nrho =%5i, nt =%5i.\n", nrho, nt);

    /* Check that enough data has been read to define coefficients. */
    if ( nt<4 || nrho<4 ) {
        printf("\n ...Bad parameter value(s): nt = %i, nrho = %i\n",
               nt, nrho);
        retval = -1;
        goto Abort;
    }

/*-------------------------------------------------------------*/
/* Allocate LIP interpolation objects, store data in them, */
/* and compute interpolation coefficients.                 */

    job_flag = 3;  /* Do full coefficient setup. */

    /* Note that the xname and yname values were chosen specifically */
    /* for the provided data set alplog, which has logged variables. */

    int_type = LIP_HERM;
    retval = lip_setup_interp( &interp_herm, "log(rho)", nrho, rho,
                               "log(T)", nt, t, fname, f, int_type,
                               job_flag );

    /* Should check value of retval and take appropriate action. */

    int_type = LIP_MONO;
    retval = lip_setup_interp( &interp_mono, "log(rho)", nrho, rho,
                               "log(T)", nt, t, fname, f, int_type,
                               job_flag );
```

```
    /* Should check value of retval and take appropriate action. */

/*----------------------------------------*/
/* Set up variables for evaluating function */
/* and derivatives on data mesh.           */

    npts = nrho*nt;  /* Total number of data points. */
    rhoval = NULL;
    rhoval = FMAKE_N( Real8, npts, "SAMPLE:rhoval" );
    tval = NULL;
    tval = FMAKE_N( Real8, npts, "SAMPLE:tval" );
    p1val = NULL;
    p1val = FMAKE_N( Real8, npts, "SAMPLE:p1val" );
    dp1dr = NULL;
    dp1dr = FMAKE_N( Real8, npts, "SAMPLE:dp1dr" );
    dp1dt = NULL;
    dp1dt = FMAKE_N( Real8, npts, "SAMPLE:dp1dt" );
    p2val = NULL;
    p2val = FMAKE_N( Real8, npts, "SAMPLE:p2val" );
    dp2dr = NULL;
    dp2dr = FMAKE_N( Real8, npts, "SAMPLE:dp2dr" );
    dp2dt = NULL;
    dp2dt = FMAKE_N( Real8, npts, "SAMPLE:dp2dt" );
    if (  (rhoval==NULL) || (tval==NULL) ||
          (p1val==NULL) || (dp1dr==NULL) || (dp1dt==NULL) ||
          (p2val==NULL) || (dp2dr==NULL) || (dp2dt==NULL) ) {
        printf ("Trouble allocating storage for test arrays.\n");
        goto Done;
    }

    /* Pick up mesh in a 2-D array for evaluation. */
    k = 0;
    for (i=0; i<nrho; i++) {
        for (j=0; j<nt; j++) {
            rhoval[k] = rho[i];
            tval[k] = t[j];
            k++;
        }
    }
    if (k != npts) {
        printf ("Trouble setting up test mesh.");
        printf ("  Expect k = %i; got k = %i\n", npts, k);
        goto Done;
    }

/*---------------------------------------------------------------*/
/* Evaluate both interpolants and derivatives on the data mesh. */

    calcf=TRUE;  /* Calculate function values. */
    calcdr=TRUE; /* Calculate df/drho values. */
    calcdt=TRUE; /* Calculate df/dt values. */

    retval = lip_evalu_bivar(interp_herm, LIP_HERM, extr_flag,
                             rhoval, tval, npts, calcf, p1val,
                             calcdr, dp1dr, calcdt, dp1dt);
    /* Should check value of retval and take appropriate action. */

    retval = lip_evalu_bivar(interp_mono, LIP_MONO, extr_flag,
```

```
                            rhoval, tval, npts, calcf, p2val,
                            calcdr, dp2dr, calcdt, dp2dt);
    /* Should check value of retval and take appropriate action. */

/*---------------------------------------------------------------*/
/*  Loop over input mesh and compare computed results with data, */
/*  and also compare BIHERM with BIMOND at the data points.      */

    nbad1 = 0; /* Number of points where BIHERM values fail test. */
    nbad2 = 0; /* Number of points where BIMOND does not match. */
    k = 0;
    for (i=0; i<nrho; i++) {
        for (j=0; j<nt; j++) {

            error = fabs( f[j*nrho+i] - p1val[k] );
            if (error != 0.)  error /= maxabs( f[j*nrho+i], p1val[k] );
            if ( error > ERRTOL ) nbad1++;

          /* Compare with BIMOND interpolant. */
            error = fabs( p2val[k] - p1val[k] );
            if (error != 0.)  error /= maxabs( p2val[k], p1val[k] );
            if ( error > ERRTOL ) nbad2++;
            k++;

        }  /* End j-loop. */
    }  /* End i-loop. */

    /* Print summary of test results. */

    printf ("\n Tolerance for meshpoint accuracy tests = %e.\n", ERRTOL);
    printf (" %5i values of BIHERM interpolant failed to agree.\n",
            nbad1);
    printf (" %5i values of BIMOND interpolant failed to agree.\n",
             nbad2);

/*---------------------------------------------------------------*/
/*  Loop over mesh and look for negative derivative values. */
/* (A monotone interpolant will have positive derivatives.) */

    nbad1 = 0; /* Number of negative p1 derivative values. */
    nbad2 = 0; /* Number of negative p2 derivative values. */
    k = 0;
    for (i=0; i<nrho; i++) {
        for (j=0; j<nt; j++) {

            if ( dp1dr[k] < 0. )  nbad1++;
            if ( dp1dt[k] < 0. )  nbad1++;

            if ( dp2dr[k] < 0. )  nbad2++;
            if ( dp2dt[k] < 0. )  nbad2++;

            k++;

        }  /* End j-loop. */
    }  /* End i-loop. */

    /* Print summary of derivative test results. */
```

```
   printf ("\n For monotonicity, all derivative should be positive.\n");
   printf (" %5i values of BIHERM derivative at data points < 0.\n", nbad1);
   printf (" %5i values of BIMOND derivative at data points < 0.\n", nbad2);

/*-------------------------------------------------------------*/
/*  The BIHERM interpolant is known to be nonmonotonic on      */
/*  mesh box (4,0).  Pick up several interior points which     */
/*  illustrate this point and evaluate both interpolants       */
/*  at those points.                                           */

    drho = rho[5] - rho[4];
    dt = t[1] - t[0];

    k = 0;
    for (i=1; i<4; i++) {
        rhosave = rho[4] + i*0.25*drho;
        for (j=1; j<4; j++) {
            rhoval[k] = rhosave;
            tval[k] = t[0] + j*0.25*dt;
            k++;
        }  /* End j-loop. */
    }  /* End i-loop. */

    npts = k;
    printf ("\n Evaluating at %i points, the quarter-points of mesh\n",
            npts);
    printf ("    box with lower-left corner at (rho,t)=(%.2f,%.2f).\n",
            rho[4], t[0]);

    /* Note that the calc flags are the same as before. */

    fflush (stdout);
    retval = lip_evalu_bivar(interp_herm, LIP_HERM, extr_flag,
                             rhoval, tval, npts, calcf, p1val,
                             calcdr, dp1dr, calcdt, dp1dt);
    /* Should check value of retval and take appropriate action. */

    fflush (stdout);
    retval = lip_evalu_bivar(interp_mono, LIP_MONO, extr_flag,
                             rhoval, tval, npts, calcf, p2val,
                             calcdr, dp2dr, calcdt, dp2dt);
    /* Should check value of retval and take appropriate action. */

    printf ("\n  rho     T        p1       dp1/drho   dp1/dT");
    printf ("      p2       dp2/drho   dp2/dT\n");
    for (k=0; k<npts; k++) {
        printf ("%6.4f%8.4f%11.3e%11.3e%10.3e%11.3e%11.3e%10.3e\n",
                rhoval[k], tval[k],
                p1val[k], dp1dr[k], dp1dt[k],
                p2val[k], dp2dr[k], dp2dt[k]);
    }

/*------------------*/

Done:
    printf("\n");
    fflush(stdout);
```

```
/* Free test variables */

    if ( rhoval != NULL )  SFREE( rhoval );
    if (   tval != NULL )  SFREE( tval );
    if (  p1val != NULL )  SFREE( p1val );
    if (  dp1dr != NULL )  SFREE( dp1dr );
    if (  dp1dt != NULL )  SFREE( dp1dt );
    if (  p2val != NULL )  SFREE( p2val );
    if (  dp2dr != NULL )  SFREE( dp2dr );
    if (  dp2dt != NULL )  SFREE( dp2dt );

/* Free the LIP_interp objects. */

    /* Free interp_herm. */
    retfree = lip_free_interp( &interp_herm );
    /* Should check value of retfree and take appropriate action. */

    /* Free interp_mono. */
    retfree = lip_free_interp( &interp_mono );
    /* Should check value of retfree and take appropriate action. */

/* Free space allocated by readeos. */

Abort:  /* Transfer point for errors during setup. */
    SFREE( rho );
    SFREE( t );
    SFREE( f );

    return retval;

}
/********************/
/* End of main code */
/********************/
```

# 9. Possible Enhancements

### *9.1. Lookup improvements*

Since EOS tabulation points are logarithmically spaced, it may be possible to further speed up the lookup phase by introducing a hash table or other device. It will be necessary to do this without incurring the expense of a logarithm or exponential call during evaluation. (Note: This may be out of place in a general interpolation library.)

### *9.2. Providing for user-supplied derivatives*

Both the 12-term bicubic and the bicubic Hermite form use derivative values during coefficient setup. If such values are available, a facility should be provided to let them be supplied, rather than estimating them from the data.

### *9.3. Allowing decreasing mesh arrays*

At present LIP requires that both independent variable arrays be strictly increasing. Other than the major coding changes that would be required, there is no inherent reason not to allow either or both of the mesh arrays to be strictly *de*creasing, instead.

### *9.4. Inversion in either independent variable*

Historically, only inversion in the second independent variable (which is T for LEOS data) has been supported. It has been proposed that inversion in the first independent variable also be included in LIP, with appropriate safeguards for possible non-monotonic data.

# References

[1] Fritsch, Frederick N., The LEOS Interpolation Package, Third Edition, UCRL-ID-148544-Rev.1 (March 12, 2003).

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[3] Carlson, R.E., and F.N. Fritsch, "An algorithm for monotone piecewise bicubic interpolation", SIAM J. Numer. Anal., Vol. 26, No. 1 (February 1989), pp.230–238. [The associated Fortran code, `BIMOND3`, was documented in UCID-21143 (August 1987).]

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[5] Chase, Lila, EOS4 User Manual, Internal Report UCIR-1436a, Rev. 33 (July 7, 1999).

[6] Brown, S.A, and D. Braddy, PACT Users Guide, UCRL-MA-112087 (1993).

[7] Kerley, Gerald I., Rational Function Method of Interpolation, Informal Report LA-6903-MS, Los Alamos National Laboratory (August 1977).

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# Appendix A. Values for LIP_interp Fields

This appendix lists the currently allowable values for certain fields in a `LIP_interp` object. These are defined in `LIP_setup.h`.

The `setup_type` (setup type) field may have the following values:

`LSU_UNINIT` : Uninitialized.

`LSU_INIT` : Initialized, but no data stored.

`LSU_DATA` : Only data provided.

`LSU_1DER` : Data + 1 derivative provided. [1-D data only]

`LSU_2DER` : Data + 2 derivatives provided. [2-D data only]

`LSU_3DER` : Data + 3 derivatives provided (both first partials plus twists). [2-D data only]

`LSU_COEF` : Full coefficient setup done.

These are defined in an `enum`, and have increasing values moving down the list.

The `int_type` (interpolation type) field may have the following values:

`LIP_INVALID` : Invalid, but initialized.

`LIP_LIN` : (Bi)linear interpolation. (See Section 2.)

`LIP_CUB` : "Standard" (bi)cubic interpolation. (See Section 3.)

`LIP_CUBM` : Modified bicubic interpolation (2-phase data). (See Section 3.3.)

`LIP_HERM` : (Bi)cubic Hermite interpolation. (See Section 4.)

`LIP_MONO` : Monotone (bi)cubic interpolation. (See Section 4.3.)

`LIP_QUAD` : Biquadratic interpolation. (See Section 5.)

`LIP_RAT` : (Bi)rational interpolation. (See Section 6.)

These are defined in an `enum`, and have increasing values moving down the list.

# Appendix B. Adding a New Interpolation Method

The purpose of these notes is to discuss what is required for an interpolation method to be appropriate for LIP and to describe how to add such a new interpolator.

**1. What kinds of interpolators can be supported?**

The Livermore Interpolation Package (LIP) exists to support data provided on a two-dimensional rectangular mesh; namely, f(x,y): $x = x_0, x_1, ..., x_{nx-1}$; $y = y_0, y_1, ..., y_{ny-1}$. (Subscripting is from zero to be consistent with the C code.) Thus any interpolation method based on function (and possibly derivative) values on such a mesh is a potential candidate for a LIP interpolator. For full support, the following must be possible:

- The interpolation scheme can be factorized into a setup and an evaluation phase. The former computes a fixed number, nbasfcns, of interpolation coefficients for each mesh box. (Although we refer to *nbasfcns*, meaning *number of basis functions*, it is not required that the interpolant actually be a linear combination of basis functions.) At setup time these are stored in a coefficient array of size (nx–1)*(ny–1)*nbasfcns, where the original data mesh is nx by ny.

  Alternatively if only partial setup (see Section 1.4) is done, the evaluation phase must be able to compute the coefficient array for the current mesh box (or values of the interpolant) from the available data.

- A one-dimensional analog of the method, which is compatible with the 2-D method in the sense of Section 1.2, must exist. *Caution*: For this to work best, the "bixxx" functional form needs to be symmetric, so that the same univariate form applies to interpolation in either variable. That is, $f(x,y_{const}) = g(x)$ and $f(x_{const},y) = g(y)$, with the same univariate functional form g(x) – with different coefficients, of course.

- It must be possible to provide for inverse interpolation, as discussed in Section 1.8.

As a concrete example of a symmetric functional form, consider

$$\begin{aligned} f(x,y) \;=\; & ( c_{00} + c_{10}\, x + c_{20}\, \ln(x) + c_{30}\, 1/x ) \\ & + ( c_{01} + c_{11}\, x + c_{21}\, \ln(x) + c_{31}\, 1/x )\, y \\ & + ( c_{02} + c_{12}\, x + c_{22}\, \ln(x) + c_{32}\, 1/x )\, \ln(y) \\ & + ( c_{03} + c_{13}\, x + c_{23}\, \ln(x) + c_{33}\, 1/x )\, 1/y \text{ , where } x>0,\ y>0. \end{aligned}$$

This has nbasfcns = 16, the same as `LIP_HERM`. Obviously, if we fix x, this reduces to

$$\begin{aligned} g(y) \;=\; & a_1 + b_1\, y + c_1\, \ln(y) + d_1\, 1/y \text{ , where} \\ & a_1 = c_{00} + c_{10}\, x + c_{20}\, \ln(x) + c_{30}\, 1/x \text{ ,} \\ & b_1 = c_{01} + c_{11}\, x + c_{21}\, \ln(x) + c_{31}\, 1/x \text{ ,} \\ & c_1 = c_{02} + c_{12}\, x + c_{22}\, \ln(x) + c_{32}\, 1/x \text{ ,} \\ & d_1 = c_{03} + c_{13}\, x + c_{23}\, \ln(x) + c_{33}\, 1/x \text{ .} \end{aligned}$$

Similarly, if we fix y, this reduces to

$$g(x) = a_2 + b_2\, x + c_2\, \ln(x) + d_2\, 1/x \text{ , where}$$

$$a_2 = c_{00} + c_{01}\, y + c_{02}\, \ln(y) + c_{03}\, 1/y \text{ ,}$$
$$b_2 = c_{10} + c_{11}\, y + c_{12}\, \ln(y) + c_{13}\, 1/y \text{ ,}$$
$$c_2 = c_{20} + c_{21}\, y + c_{22}\, \ln(y) + c_{23}\, 1/y \text{ ,}$$
$$d_2 = c_{30} + c_{31}\, y + c_{32}\, \ln(y) + c_{33}\, 1/y \text{ .}$$

Thus f has the desired symmetry property. The univariate analog has nbasfcns = 4.

**2. Adding a new interpolation method to LIP.**

In this section we refer to the new method as "bixxx interpolation", and its 1-D analog as "xxx interpolation".

Use existing functions in the files mentioned below as a guide to the assumed calling sequences. It is taken for granted that calling sequence documentation will be updated as necessary to reflect the new method. (A skeleton for the LIP standard prologue format is in file `lip/aux_source/skeleton`.)

1. Choose an `int_type` name `LIP_XXX` to designate bixxx interpolation and add its definition to `LIP_setup.h`. Note that this must be different from all previously defined interpolation type designators. Be sure to update `lip_get_nbasfcns` in `lip_setup_c` to test for this new `int_type`. (This may also require a change to `nbasfcns.c` and/or its output `nbas_out` in `lip/test/liptest`.)
2. Write a function `lip_evalu_bixxx` that evaluates a previously set-up bixxx interpolant at an array of points. Add this to file `lip_eval2D.c`. Add a suitable call to it to `leos_evalu_box` in this file.
3. Write a function `lip_evalu_xxx` which evaluates a previously set-up xxx interpolant at an array of points. Add this to file `lip_eval1D.c`. Add a suitable call to it to `lip_evalu_cell` in this file.
4. Write a function `lip_setup_bixxx` that sets up the full coefficient array for bixxx interpolation. Add this to file `lip_coeff.c`. Add a suitable call to it to `leos_calc_coeff` in this file. (This is not necessary if the method is only implemented for the "partial setup" mode.)
5. Also write a function `lip_setup_xxx` that sets up the coefficient array for (univariate) xxx interpolation. Add this to file `lip_coeff.c` as well, and add a suitable call to it to `leos_calc_coeff` in this file. (Again, may not be necessary.)
6. Write a function `lip_inv_bixxx` which implements inverse bixxx interpolation in full coefficient setup mode, if appropriate. Add this to file `lip_inverse.c`. Add a suitable call to it to `lip_inv_coeff` in this file. If partial setup is supported, add a function with a similar name to support it, via a new call from `lip_inv_partial`. (If neither is done, inversion may still be possible by using `lip_inv_general`.)

7. Oh, yes! *Don't forget to change the LIP version number and date* in file `configure.in` (refer to the `README` file in directory `lip/config`). (To date, no policy has been established for version numbering, but this is a significant enough change that at least the first digit after the decimal point should be incremented.)
8. Update the documentation files (in directory `lip/docs`). The tools there will be helpful here. Note that it will be necessary to update file `prologue_interp` to reflect the current status. It may also be necessary to update file `names_interp` if you wish to include the new setup functions in the document. (Of course, you will need to update the prologues of the source files to which you add the new functions mentioned above.)
9. Add a bixxx option to appropriate test codes in `lip/test`. This may require adding new input and/or output files and modifying the `Run_this` scripts to run additional cases. If appropriate, also add a new test specific to this new method.

Note that items 2–6 will require addition of new prototypes to `LIP_proto.h`.

# Appendix C. Data Read Function for Example

Following is the listing of the source code for function `readeos`, used by the example program of Section 7 to read its input data. The assumed format of the file is described in the initial comments. (We have omitted initial `#include`'s that don't aid understanding of the code.)

```
#include "LIP_macros.h"  /* For FMAKE_N. */
#include "LIP_Ftype.h"   /* For LIP data type definitions. */

extern char errmsg[];   /* Link to test global error message string. */

/*****************************/
/* Start of function readeos */
/*****************************/
Integer readeos(const char *filename,
                Integer *nx, Real8 **x, Integer *ny, Real8 **y,
                Real8 **f, char *fname)

/*************************************************************************
**************************************************************************
*  Function to read a function from an LEOS 3-column data file.
*  (See note below on assumed format of the input file.)
*
   (Omitted comments on how readeos differs from read_eos.)
*
*  This function allocates array storage internally, after reading nx
*  and ny.  It is the responsibility of the calling program to call
*  SFREE for x, y, f when finished using them.  Note that to get the
*  connection right, these arrays are treated as pointers to pointers
*  here, and the ADDRESSES of the external arrays need to be sent in
*  where those arrays appear in the call list.
*
* Input variables:
*     filename  Name of the file to be read.
*
* Output variables:
*     nx        Number of x-values.
*     x         The x-values.
*     ny        Number of y-values.
*     y         The y-values.
*     f         The f-values.
*     fname     Will be the name of the dependent variable as read from
*               the file.
*  If there was trouble reading the data, the return value will be
*  negative.  On succesesful return, the data are stored in f in the
*  order required by LIP; that is, f[j*nx+i] is the value at point
*  x(i), y(j).
*
* Return value:  The return value, retval, should be zero.
*   The possible fatal error returns are:
*     retval =   -1 : cannot open input file.
*     retval =   -2 : problem scanning (fname,ny,nx) line for data set.
*     retval =   -3 : nx and/or nx <= 0.
```

```
*     retval =  -10 : bad y-value detected (nonrectangular mesh?).
*     retval = -100 : Trouble allocating memory.
*     retval = -200 : EOF encountered while reading Data ID Block.
*     retval = -201 : EOF encountered before end of a data set.
*  All error indications will result in a message to the global error
*  message string errmsg, as well.
*
* Assumed data format:
*  The first line of each table contains fname and two integers, in the
*  order ny and nx.  The fname field is assumed to be at most eight
*  characters.  For historical reasons, the second dependent variable
*  (temperature for EOS data) is read before the first (EOS density).
*  This line is read via sscanf with format "%s %i %i".
*  The data then follow as y, x, f triples, with all the x-values for
*  a given y together.  (Again, note the order!)
*
*  This version allows a data ID block to be given before the data itself.
*  The first line of the block must be "*Begin ID Block" and the last line
*  of the block must be "*End ID Block".  The case of all letters must be
*  exactly as indicated here.  Any lines of text the creator of the table
*  wishes to use to identify the data may appear between these two lines.
*
*  This version looks for a file named "read_verbose".  If it exists, the
*  x and y arrays are printed, as well as the first and last values of
*  the dependent variable.  The data ID block, if present, will also be
*  printed in this case.
*
* Change record:
* (yymmdd means 20yy/mm/dd)
*  080806  Initial implementation by Fred N. Fritsch, LEOS Development
*          Team, from existing read_eos.
*  080812  Corrected errors in initial conversion and omitted argument
*          fread. (FNF)
*  080812  Modified to print error messages to errmsg, not stdout. (FNF)
*
************************************************************************
************************************************************************/
 {

/* Declare local variables */

   FILE *infile;
   char line[MAXLINE], invar[]="(none)";
   Integer i, j, retval;
   Real8   fin, xin, yin;
   Logical idblock, verbose;


/* Begin executable statements */
/* =========================== */

/* Look for file "read_verbose" and set flag verbose accordingly. */

   verbose = FALSE;
   if ( fopen("read_verbose", "r") != NULL )  verbose = TRUE;

/* Open the file to be read. */
```

```
   infile = fopen(filename, "r");
   if (infile == NULL) {
      sprintf(errmsg,
              "File  %s  does  not  exist  or  is  not  readable.\n",
filename);
      return (-1);
   }

/* Initialize. */

   idblock = FALSE;

   *x = (Real8 *) NULL;
   *y = (Real8 *) NULL;
   *f = (Real8 *) NULL;

Continue10:
      if (fgets(line, MAXLINE, infile) == NULL) {
         if (idblock) goto Read_error;
         else         goto Normal_exit;
      }

   /* Process optional data ID block. */

      if (strncmp(line, "*Begin ID Block", 15) == 0)  idblock = TRUE;
      if (idblock) {
         if (verbose)  printf(" %s", line);
         if (strncmp(line, "*End ID Block", 13) == 0) {
            idblock = FALSE;
            if (verbose)  printf(" \n");
         }
         goto Continue10;
      }

   /* Read initial data line (fname,ny,nx). */

      if (sscanf(line, "%s %i %i", fname, ny, nx) == EOF) {
         sprintf(errmsg,
                 " ERROR: Illegal initial data line:  %s\n", line);
         return (-2);
      } else {
         printf(" Reading variable %s", fname);
         printf(":   ny =%5i", *ny);
         printf(", nx =%5i\n", *nx);
         fflush(stdout);
      }
      if ( (*ny <= 0) || (*nx <= 0) ) {
         sprintf(errmsg,
                 "   ERROR: Bad ny=%i or nx=%i\n", *ny, *nx);
         sprintf(errmsg, "\t***  Aborting EOS read.\n");
         return (-3);
      }

   /* Allocate space for mesh variables. */

      *x = FMAKE_N(Real8, (*nx), "Readeos:x");
      *y = FMAKE_N(Real8, (*ny), "Readeos:y");
      if (*x == NULL || *y == NULL) goto Allocate_error;
```

```
/* Allocate space for function being read. */

   *f = FMAKE_N(Real8, (*nx)*(*ny), "Readeos:f");
   if (*f == NULL) goto Allocate_error;

/* Loop over y-values. */

   for (j = 0; j < *ny; j++) {

  /* Loop over x-values. */

      for (i = 0; i < *nx; i++) {
         if (fscanf(infile,"%le", &yin) == EOF) {
            strcpy(invar, "yin");
            goto Read_error;
         }
         if (fscanf(infile,"%le", &xin) == EOF) {
            strcpy(invar, "xin");
            goto Read_error;
         }
         if (fscanf(infile,"%le", &fin) == EOF) {
            strcpy(invar, "fin");
            goto Read_error;
         }
         if (i > 0) {
            if (yin != (*y)[j]) {
               sprintf(errmsg,
                       " Bad y-value.  Read %e; expected %e\n",
                       yin, (*y)[j]);
               retval = -10;
               goto Clean_up;
            }
         }
       /* Don't store y if already stored. */
         if (i == 0) {
            (*y)[j] = yin;
         }
       /* Store x. */
         (*x)[i] = xin;
       /* Store f. */
         (*f)[j*(*nx)+i] = fin;
      }
   }

   printf(" Finished reading %s data.\n", fname);
   if (verbose) {
      printf(" x-values:\n    ");
      for (i = 0;  i < *nx; i++) {
         printf("%15.7E", (*x)[i]);
         if (i == *nx-1) printf("\n");
         else if (i%5 == 4) printf("\n    ");
      }
      printf(" y-values:\n    ");
      for (j = 0;  j < *ny; j++) {
         printf("%15.7E", (*y)[j]);
         if (j == *ny-1) printf("\n");
         else if (j%5 == 4) printf("\n    ");
```

```
         }
         printf(" First and last %s-values:\n", fname);
         printf("    %15.7E%15.7E\n", (*f)[0], (*f)[(*ny-1)*(*nx)+*nx-1]);
      }
      printf("\n");

      /* Get rid of dangling end-of-line. */
      if (fgets(line, MAXLINE, infile) == NULL) goto Read_error;

/*  Normal exit. */

Normal_exit:
   printf(" Done reading data from file %s\n", filename);
   retval = 0;
   goto Clean_up;

/*  Error exits. */

Allocate_error:
   sprintf(errmsg,
           " ERROR: Cannot allocate space for one or more arrays.\n");
   retval = -100;
   goto Clean_up;

Read_error:
   if (idblock) {
      sprintf(errmsg, " ERROR: EOF while reading data ID block.\n");
      sprintf(errmsg, "       Missing '*End ID Block' line?\n");
      retval = -200;
   } else {
      sprintf(errmsg,
              " ERROR: EOF before end of data while reading %s for %s\n",
              invar, fname);
      retval = -201;
   }

Clean_up:
   /* Note: cannot free arrays here, because they are to be accessed */
   /*       and used by calling program.                             */

   /* The following error message should never appear. */
   if ( (*x == NULL) || (*y == NULL) || (*f == NULL) ) {
      printf(" ERROR: One or more NULL array pointers in readeos.\n");
   }

   return(retval);
}
/*************************/
/* End of function readeos */
/*************************/
```

# Appendix D. Input File for Example

Following is the data file `alplog` read by the example program in Section 7. These data are increasing in both variables, although clearly not strictly increasing, for there are sections where the values are independent of ρ (second column). Note that the name of the file stands for "aluminum pressure with all variables logged". The "truncated" in the initial line of the ID Block means (1) this is but a small segment of a much larger EOS table and (2) the values have been truncated to two digits after the decimal point.

```
*Begin ID Block
       Truncated section of aluminum EOS table
This is the sample data set distributed with BIMOND3, converted
to the format expected by readeos. (FNF 5/24/2001)
Note that the data columns are log(T), log(rho), log(P).
*End ID Block
log(P)   6    10
     -2.30                -0.07               -34.54
     -2.30                 0.33               -34.54
     -2.30                 0.55               -34.54
     -2.30                 0.69               -34.54
     -2.30                 0.84               -34.54
     -2.30                 0.93               -34.54
     -2.30                 0.98                -3.06
     -2.30                 1.02                -2.86
     -2.30                 1.08                -2.37
     -2.30                 1.13                -1.89
     -1.61                -0.07               -13.82
     -1.61                 0.33               -13.82
     -1.61                 0.55               -13.82
     -1.61                 0.69               -13.82
     -1.61                 0.84               -13.82
     -1.61                 0.93                -2.68
     -1.61                 0.98                -2.28
     -1.61                 1.02                -1.92
     -1.61                 1.08                -1.60
     -1.61                 1.13                -1.30
     -0.92                -0.07               -10.10
     -0.92                 0.33               -10.10
     -0.92                 0.55               -10.10
     -0.92                 0.69               -10.10
     -0.92                 0.84                -2.52
     -0.92                 0.93                -1.88
     -0.92                 0.98                -1.63
     -0.92                 1.02                -1.39
     -0.92                 1.08                -1.17
     -0.92                 1.13                -0.95
     -0.51                -0.07                -7.26
     -0.51                 0.33                -7.26
     -0.51                 0.55                -7.26
     -0.51                 0.69                -4.82
     -0.51                 0.84                -2.22
     -0.51                 0.93                -1.56
```

# Appendix D. Input File for Example

```
-0.51                0.98               -1.32
-0.51                1.02               -1.10
-0.51                1.08               -0.90
-0.51                1.13               -0.71
-0.22               -0.07               -5.66
-0.22                0.33               -5.66
-0.22                0.55               -4.88
-0.22                0.69               -3.34
-0.22                0.84               -1.98
-0.22                0.93               -1.41
-0.22                0.98               -1.15
-0.22                1.02               -0.92
-0.22                1.08               -0.72
-0.22                1.13               -0.54
 0.                 -0.07               -4.53
 0.                  0.33               -4.13
 0.                  0.55               -3.35
 0.                  0.69               -2.73
 0.                  0.84               -1.78
 0.                  0.93               -1.28
 0.                  0.98               -1.05
 0.                  1.02               -0.81
 0.                  1.08               -0.60
 0.                  1.13               -0.41
```

# Appendix E. Output File for Example

Following is the result of running the example program in Section 7 with the input data given in Appendix D. Note three pieces of evidence that the BIHERM interpolant $p_1$ is not monotonic, even though the data are, but the BIMOND interpolant $p_2$ is monotonic. First, six negative derivative values were found when $p_1$ was evaluated on the data mesh, but none for $p_2$. Second, in the mesh box (4,0) chosen for special study we find one negative value for $\partial p_1/\partial \rho$, but none for $p_2$. Finally, we see that

$$p_1(0.8850,-2.1275) - p_1(0.8625,-2.1275) = (-29.67) - (-29.60) = -0.07,$$
$$p_1(0.9075,-2.1275) - p_1(0.8850,-2.1275) = (-27.52) - (-29.67) = +2.15,$$

so $p_1$ clearly is not monotonic in the first variable!

```
         LIP sample code
        -----------------

 Type file name.
alplog

 Reading variable log(P):   ny =    6, nx =   10
 Finished reading log(P) data.

 Done reading data from file alplog

 readeos returned nrho =   10, nt =    6.

        Results for log(P) table from file alplog

 Tolerance for meshpoint accuracy tests = 1.000000e-14.
     0 values of BIHERM interpolant failed to agree.
     0 values of BIMOND interpolant failed to agree.

 For monotonicity, all derivative should be positive.
     6 values of BIHERM derivative at data points < 0.
     0 values of BIMOND derivative at data points < 0.

 Evaluating at 9 points, the quarter-points of mesh
    box with lower-left corner at (rho,t)=(0.84,-2.30).
```

# Appendix E. Output File for Example

| rho | T | p1 | dp1/drho | dp1/dT | p2 | dp2/drho | dp2/dT |
|---|---|---|---|---|---|---|---|
| 0.8625 | -2.1275 | -2.960e+01 | -3.121e+01 | 4.602e+01 | -2.721e+01 | 8.768e+01 | 4.156e+01 |
| 0.8625 | -1.9550 | -2.220e+01 | 6.974e+01 | 3.967e+01 | -2.048e+01 | 1.347e+02 | 3.574e+01 |
| 0.8625 | -1.7825 | -1.596e+01 | 1.265e+02 | 3.251e+01 | -1.516e+01 | 1.489e+02 | 2.510e+01 |
| 0.8850 | -2.1275 | -2.967e+01 | 3.579e+01 | 6.190e+01 | -2.480e+01 | 1.171e+02 | 5.211e+01 |
| 0.8850 | -1.9550 | -2.012e+01 | 1.161e+02 | 4.885e+01 | -1.677e+01 | 1.802e+02 | 4.043e+01 |
| 0.8850 | -1.7825 | -1.280e+01 | 1.499e+02 | 3.600e+01 | -1.106e+01 | 1.993e+02 | 2.516e+01 |
| 0.9075 | -2.1275 | -2.752e+01 | 1.661e+02 | 7.083e+01 | -2.238e+01 | 8.829e+01 | 6.273e+01 |
| 0.9075 | -1.9550 | -1.693e+01 | 1.682e+02 | 5.219e+01 | -1.304e+01 | 1.365e+02 | 4.519e+01 |
| 0.9075 | -1.7825 | -9.406e+00 | 1.478e+02 | 3.537e+01 | -6.930e+00 | 1.515e+02 | 2.523e+01 |