Interaction dynamics in collisions of ions with molecules and clusters

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Appendix A

Atomic Units

The system of atomic units is based on the following definitions:

$$\hbar = 1, \tag{A.1}$$
$$m_e = 1, \tag{A.2}$$
$$e = 1, \tag{A.3}$$
$$4\pi\varepsilon_0 = 1. \tag{A.4}$$

In these definitions $\hbar$ is Planck's constant divided by 2π. The electron mass and charge are denoted by m_e and $-e$, respectively, and ε_0 is the electric permittivity of the vacuum. Units of other physical quantities may be constructed from these basic quantities. For example, the atomic unit of length, or the Bohr radius, is the following:

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = 0.529\text{Å}. \tag{A.5}$$

The atomic unit for velocity is αc, where the (dimensionless) fine structure constant α equals:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 c} = \frac{1}{137}. \tag{A.6}$$

This gives c, in atomic units, equal to 137.

Table A.1 contains some often used physical quantities and the description of one atomic unit of that particular quantity.

Table A.1: *A table containing often used physical quantities. The second column contains the SI equivalent of one atomic unit of the particular quantity in the first column. The third column contains a value in non-SI units. The last column displays the definition of the atomic unit for the quantity.*

Quantity	SI units	Alternate units	Definition
Length	$5.29177249 \times 10^{-11}$ m	0.529 Å	a_0
Time	$2.41888433 \times 10^{-17}$ s		$a_0/(\alpha c)$
Velocity	2.18769142×10^{6} m/s		αc
Mass	$9.1093897 \times 10^{-31}$ kg	0.000549 amu	m_e
Energy	4.3593×10^{-18} J	27.2 eV	$m_e(\alpha c)^2$
Charge	$1.6021773 \times 10^{-19}$ C		e
Momentum	$1.99285337 \times 10^{-24}$ kg m/s		$m_e(\alpha c)$
Angular momentum	1.0545887×10^{-34} Js		$\hbar$

Appendix B

Bicubic and Tricubic Interpolation

The hydrocarbon potential, used in chapter 4, contains correction functions, which are only known at integer values of the arguments. To make this potential continuous, these functions are interpolated using bicubic and tricubic interpolation. This appendix elaborates on these procedures.

B.1 Bicubic Interpolation

In bicubic interpolation a function of the form

$$H(x,y) = \sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij}x^i y^j \tag{B.1}$$

must be found, which interpolates values between integer points on a two-dimensional grid. This problem may be reduced to a problem on the unit square. Subsequently the solution procedure is then repeated on all patches in the domain of the function $H(x,y)$. On the unit square the problem has the form schematically shown in fig. B.1.

Bicubic interpolation of the unit square, or any other patch, requires the determination of 16 coefficients a_{ij}. These coefficients may be determined by setting up a system of 16 linearly independent equations. These equations may be obtained by equating the function values and the values of the derivatives with $H(x,y)$ and its derivatives at the node points. (B.2) to (B.17) display these equations.

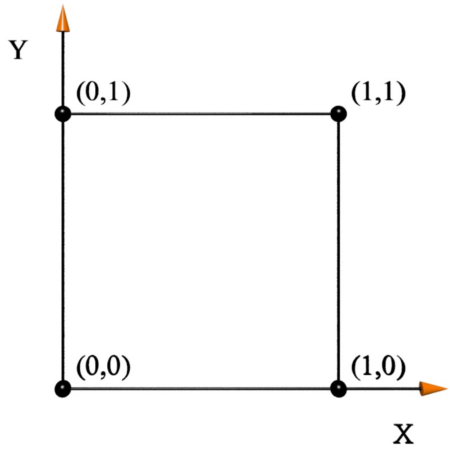

Figure B.1: *Bicubic interpolation on the unit square.*

$$
\begin{aligned}
H(0,0) &= a_{00} && \text{(B.2)}\\
H(1,0) &= a_{00}+a_{10}+a_{20}+a_{30} && \text{(B.3)}\\
H(0,1) &= a_{00}+a_{01}+a_{02}+a_{03} && \text{(B.4)}\\
H(1,1) &= \sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij} && \text{(B.5)}\\
H_x(0,0) &= a_{10} && \text{(B.6)}\\
H_x(1,0) &= a_{10}+2a_{20}+3a_{30} && \text{(B.7)}\\
H_x(0,1) &= a_{10}+a_{11}+a_{12}+a_{13} && \text{(B.8)}\\
H_x(1,1) &= \sum_{i=0}^{3}\sum_{j=0}^{3} i a_{ij} && \text{(B.9)}\\
H_y(0,0) &= a_{01} && \text{(B.10)}\\
H_y(1,0) &= a_{01}+a_{11}+a_{21}+a_{31} && \text{(B.11)}\\
H_y(0,1) &= a_{01}+2a_{02}+3a_{03} && \text{(B.12)}\\
H_y(1,1) &= \sum_{i=0}^{3}\sum_{j=0}^{3} j a_{ij} && \text{(B.13)}\\
H_{xy}(0,0) &= a_{11} && \text{(B.14)}\\
H_{xy}(1,0) &= a_{11}+2a_{21}+3a_{31} && \text{(B.15)}\\
H_{xy}(0,1) &= a_{11}+2a_{12}+3a_{13} && \text{(B.16)}\\
H_{xy}(1,1) &= \sum_{i=0}^{3}\sum_{j=0}^{3} ij a_{ij} && \text{(B.17)}
\end{aligned}
$$

If one places the coefficients a_{ij} in a vector this system of equations may be written as a matrix equation,

$$\mathbf{H} = \mathbf{M} \cdot \mathbf{a}, \tag{B.18}$$

where $\mathbf{a}$ is given by

$$\mathbf{a} = (a_{00}, a_{10}, a_{20}, a_{30}, a_{01}, a_{11}, a_{21}, a_{31}, a_{02}, a_{12}, a_{22}, a_{32}, a_{03}, a_{13}, a_{23}, a_{33})^T. \tag{B.19}$$

The vector $\mathbf{a}$ and the coefficients a_{ij} are related as

$$\mathbf{a}[1+i+4j] = a_{ij}. \tag{B.20}$$

The vector $\mathbf{H}$ is the column in front of the equality signs in eq. (B.2) to (B.17). The solution of finding the coefficients a_{ij} amounts to finding the inverse of the matrix $\mathbf{M}$ and solving for $\mathbf{a}$,

$$\mathbf{a} = \mathbf{M}^{-1} \cdot \mathbf{H}. \tag{B.21}$$

The inverse of $\mathbf{M}$ is equal to

$$\mathbf{M}^{-1} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-3 & 3 & 0 & 0 & -2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & -2 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & 3 & 0 & 0 & -2 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -2 & 0 & 0 & 1 & 1 & 0 & 0 \\
-3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & -1 & 0 \\
9 & -9 & -9 & 9 & 6 & 3 & -6 & -3 & 6 & -6 & 3 & -3 & 4 & 2 & 2 & 1 \\
-6 & 6 & 6 & -6 & -3 & -3 & 3 & 3 & -4 & 4 & -2 & 2 & -2 & -2 & -1 & -1 \\
2 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
-6 & 6 & 6 & -6 & -4 & -2 & 4 & 2 & -3 & 3 & -3 & 3 & -2 & -1 & -2 & -1 \\
4 & -4 & -4 & 4 & 2 & 2 & -2 & -2 & 2 & -2 & 2 & -2 & 1 & 1 & 1 & 1
\end{pmatrix}$$

B.2 Tricubic Interpolation

Tricubic interpolation is very similar to bicubic interpolation, described in the previous section, as both are extensions into higher dimensions of cubic interpolation. The problem in this case amounts to finding the coefficients c_{ijk} in the function $F(x,y,z)$ in eq. (B.22).

$$F(x,y,z) = \sum_{i=0}^{3}\sum_{j=0}^{3}\sum_{k=0}^{3} c_{ijk}x^i y^j z^k \tag{B.22}$$

The solution procedure described here is carried out on the unit cube. The procedure may then be repeated on other patches in the domain of $F(x,y,z)$. Similar to the case of bicubic interpolation, one sets up a system of linearly independent equations. These equations are found by equating the values of $F(x,y,z)$ and its derivatives on the eight corners of the unit cube as displayed in fig. B.2.

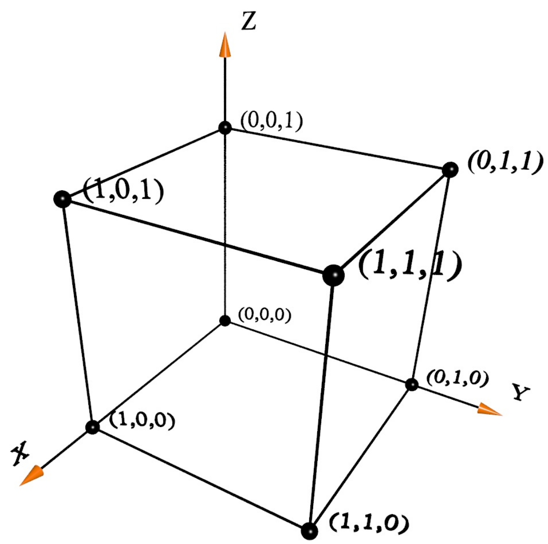

Figure B.2: *Tricubic interpolation on the unit cube.*

In tricubic interpolation there are 64 coefficients c_{ijk}. The unit cube has eight corners, so one requires eight conditions for every corner to set up a system of 64 equations. The first eight values are found by equating the function values $F(x,y,z)$ on the corners to the interpolating polynomial. 24 more conditions are found by equating the derivatives with respect to x, y and z to the respective derivatives of the interpolating polynomial. The total amount of constraints is then 32. Another 32 constraints [126] may be obtained using the cross-derivatives

f_{xy},f_{xz},f_{yz},f_{xyz}, where the sub scripts denote the variables of derivation. Other choices may be made, however, this choice leads to a solution, which is invariant under axis rotations. The set of f_{xx},f_{yy},f_{zz},f_{xyz} leads to a set of equations, which is linearly dependent.

As in the bicubic interpolation scheme, one may write this set of, in this case 64, equations in a matrix form,

$$\mathbf{F} = \mathbf{M} \cdot \mathbf{c}, \tag{B.23}$$

where $\mathbf{M}$ is a 64×64 matrix. The coefficient vector $\mathbf{c}$ has a similar form as in the bicubic case as shown in eq. (B.24),

$$\mathbf{c}[1 + i + 4j + 16k] = c_{ijk}. \tag{B.24}$$

The form of the vector holding the function and derivative values is shown in eq. (B.25).

$$\mathbf{F} = \left[F^{000\cdots111}, F_x^{000\cdots111}, F_y^{000\cdots111}, F_z^{000\cdots111}, F_{xy}^{000\cdots111}, F_{xz}^{000\cdots111}, F_{yz}^{000\cdots111}, F_{xyz}^{000\cdots111} \right]. \tag{B.25}$$

The entries of the vector $\mathbf{F}$ in eq. (B.25) each have the eight components of the corners of the unit cube as shown in the example in eq. (B.26),

$$F^{000\cdots111} = [F(0,0,0), F(1,0,0), F(0,1,0), F(1,1,0), F(0,0,1), F(1,0,1), F(0,1,1), F(1,1,1)]. \tag{B.26}$$

Similar to the case of bicubic interpolation, the coefficients c_{ijk} in tricubic interpolation may now be found by finding the inverse of the 64×64 matrix $\mathbf{M}$,

$$\mathbf{c} = \mathbf{M}^{-1} \cdot \mathbf{F}. \tag{B.27}$$

Due to its large size the matrix $\mathbf{M}^{-1}$ is not displayed here.