Quantifying Uncertainties using Interval Arithmetic

1. An Interval \( X = [a, b] \), where \( X = \{x \mid a \leq x \leq b, x \in \mathbb{R}\} \).
2. Uncertain quantities can be represented as an interval.
3. Sources of uncertainty → rounding, approximation errors
4. In a calculation, these uncertainties can be propagated on to the final result. How do we do this?
5. If the calculation involves \( +, - \), then use
   \[
   X \times Y = [\min(X,Y), \max(X,Y)]
   \]
6. More difficult challenge: How do we diagonalize matrices with interval elements? For example:
   \[
   A = \begin{bmatrix}
   1 & 2 \\
   -2 & 1
   \end{bmatrix}
   \]
   \[
   \lambda(A) = \lambda(A_+) - \rho(A), \lambda(A_+) + \rho(A)
   \]
   Where \( \lambda(A) \) and \( A \) is the centre and radius of \( A \), respectively.
8. Finding Eigenvectors of Interval Matrices requires a modified version of the Gauss-Seidel method used to solve linear system of equations.
9. Since we are able to diagonalize interval matrices, we can develop a more reliable version of several common computational chemistry methods which takes uncertainties into account.

**Example 1:**
\[
\sum_{i=1}^{1000} 0.1 = 99.99
\]
[True Solution = 100.00]

**Example 2:**
\[
f = 333.75b^4 + a^2 (11a^7b^2 - b^4 - 121b^4 - 2) + 5.5b^8 + a/(2b) = 1.172603
\]
where \( a = 77617.0, b = 33096.0 \)
[True Solution = -0.827396]

**How do we assess the impact of these uncertainties in large chemistry calculations?**

**Major Research Objectives**

1. **Analyze:** Error analysis of some commonly used methods in computational chemistry using interval arithmetic.
2. **Design:** Use interval arithmetic as a tool for designing fast algorithms with guaranteed error bounds. This method is then applied to SCF calculations on the GPU.
3. **Verify:** Use interval arithmetic to rigorously verify the results of electronic structure calculations.

**Applications**

- Fuel Cells
- Rocket Fuel Mixture
- Spectroscopy
- Reactivity
- Transition States
- Reaction Path
- Equilibrium Geometry

**Programs Developed**

1. A program for calculating the Hartree-Fock energy, orbital energies, and molecular coefficients when there are uncertain quantities. This will be used for objectives 1 and 2.
2. A program for rigorously verifying whether a set of intervals contains the correct solution of the Hartree-Fock equations in the presence of uncertainties. This will be used for objective 3.

**Author:** PETER JAMES  
PhD Candidate  
Supervisor: Alistair Rendell  
School of Computer Science  
The Australian National University