Tecniche di programmazione in chimica computazionale

Subroutines and functions

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Top-down design

- Decomposition of the main algorithm
- Logical subdivisons

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- Reusable
- Easy to read and maintain

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  instructions
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- Can return multiple results

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- Example distance.f90

Examples

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- norma_matrice.f90

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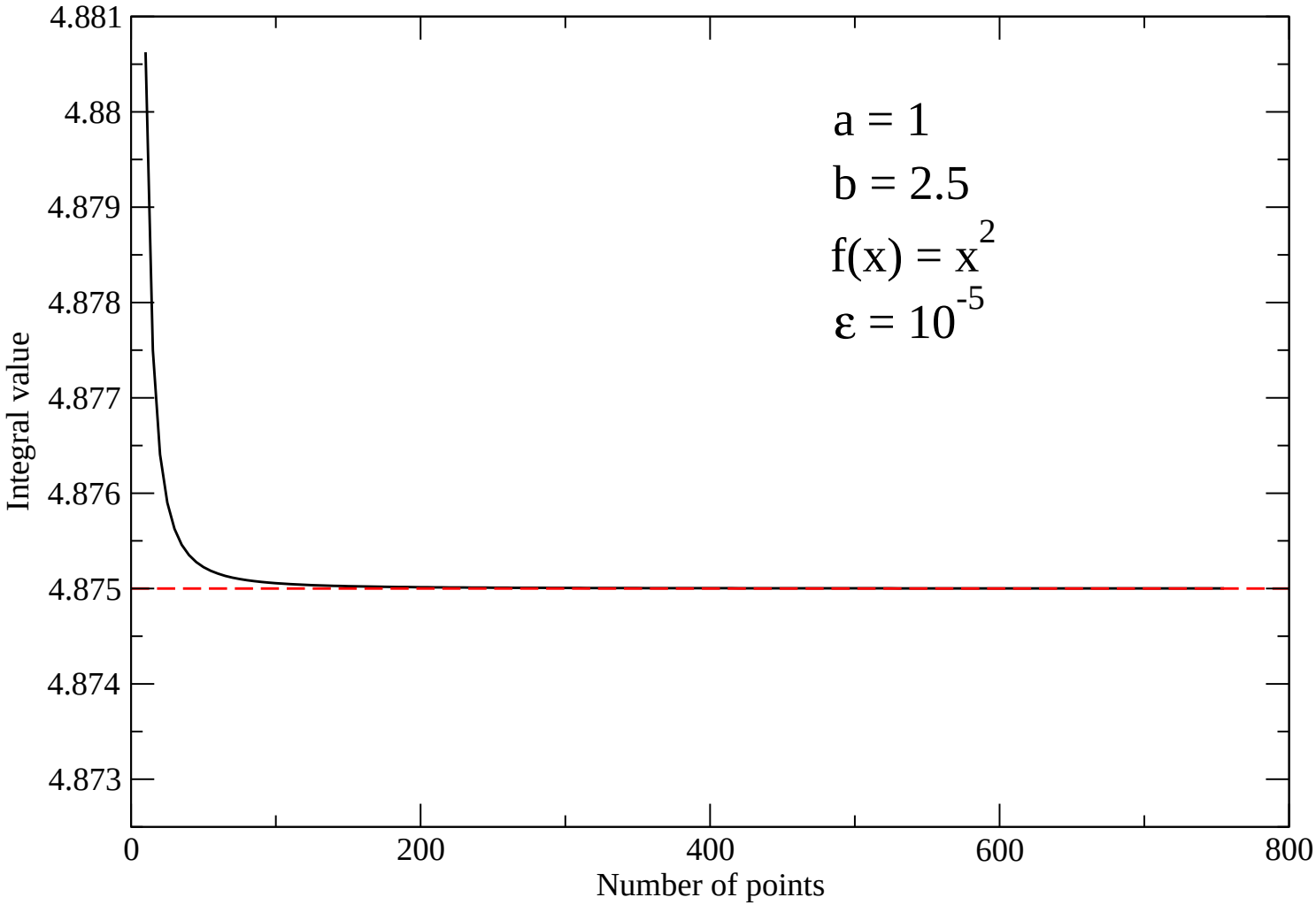
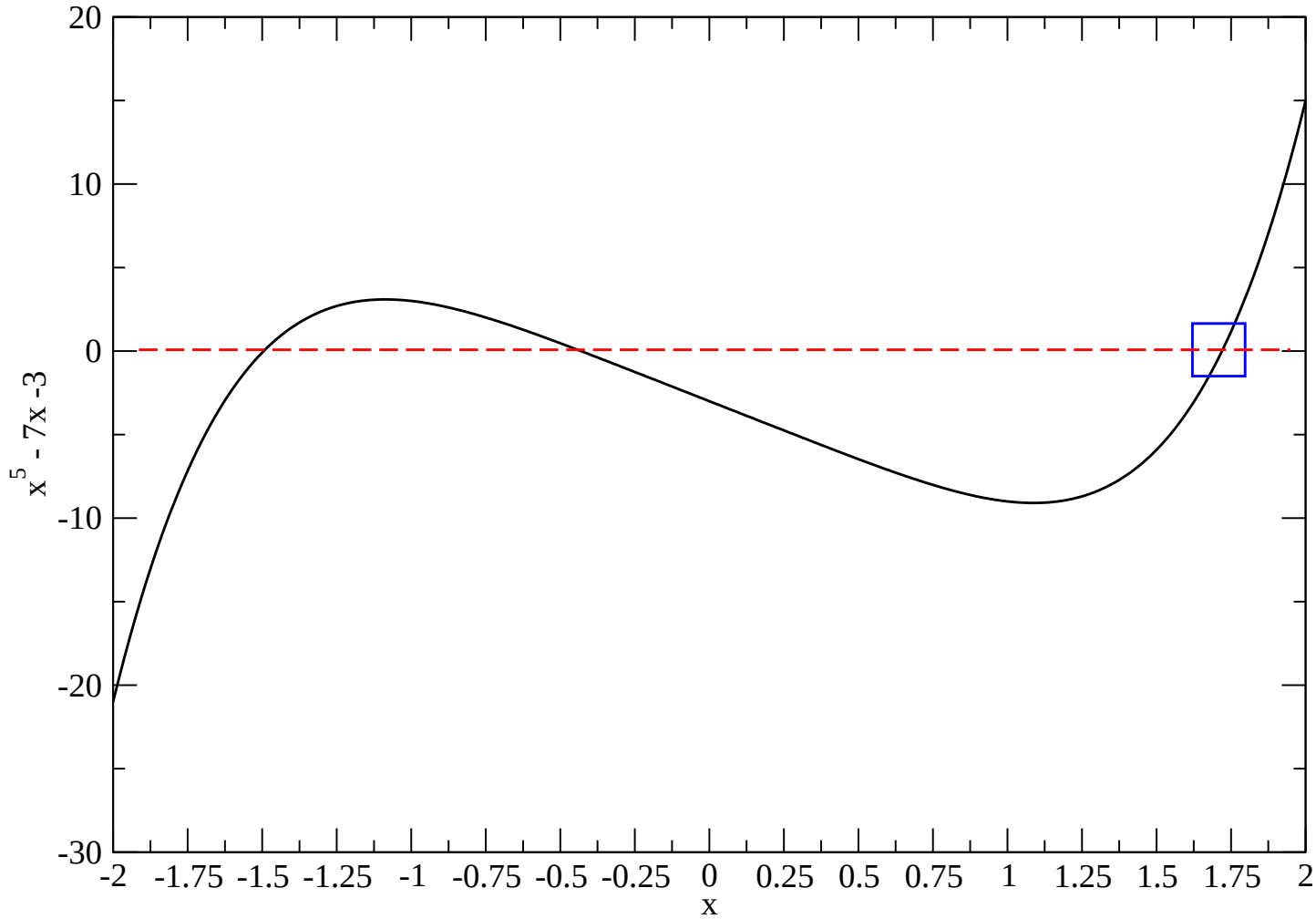
Subroutines/functions:

- media.f90

Integral f(x) = x^2



$f(x) = x^5 - 7x - 3$


20
10
0
-10
-20
-30
-2
-1.75
-1.5
-1.25
-1
-0.75
-0.5
-0.25
0
0.25
0.5
0.75
1
1.25
1.5
1.75
2
x
x^5 - 7x -3

Bubble sort

3 -1 2 4 0

Bubble sort

3 -1 2 4 0

-1 3 2 4 0

Bubble sort

3 -1 2 4 0

-1 3 2 4 0

-1 2 3 4 0

Bubble sort

3 -1 2 4 0

-1 3 2 4 0 |

-1 2 3 4 0 |

-1 2 3 4 0 |

Bubble sort

Bubble sort

3 -1 2 4 0

-1 3 2 4 0 |

-1 2 3 4 0 |

-1 2 3 4 0 |

-1 2 3 0 4 |

****

-1 2 3 0 | 4

Bubble sort

3 -1 2 4 0

-1 3 2 4 0 I

-1 2 3 4 0 I

-1 2 3 4 0 I

-1 2 3 0 4 I

****

-1 2 3 0 I 4

-1 2 3 0 I 4

Bubble sort

3 -1 2 4 0
-1 3 2 4 0 |
-1 2 3 4 0 |
-1 2 3 4 0 |
-1 2 3 0 4 |
****

-1 2 3 0 | 4
-1 2 3 0 | 4
-1 2 0 3 | 4
****

Bubble sort

3 -1 2 4 0

-1 3 2 4 0 |

-1 2 3 4 0 |

-1 2 3 4 0 |

-1 2 3 0 4 |

****

-1 2 3 0 | 4

-1 2 3 0 | 4

-1 2 0 3 | 4

****

-1 2 0 | 3 4

Bubble sort

3 -1 2 4 0
-1 3 2 4 0 |
-1 2 3 4 0 |
-1 2 3 4 0 |
-1 2 3 0 4 |
****

-1 2 3 0 | 4
-1 2 3 0 | 4
-1 2 0 3 | 4
****

-1 2 0 | 3 4
-1 0 2 | 3 4
****

Bubble sort

3 -1 2 4 0
-1 3 2 4 0 |
-1 2 3 4 0 |
-1 2 3 4 0 |
-1 2 3 0 4 |
****

-1 2 3 0 | 4
-1 2 3 0 | 4
-1 2 0 3 | 4
****

-1 2 0 | 3 4
-1 0 2 | 3 4
****

-1 0 | 2 3 4