Julia language for computational chemists

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Course details

Dates: June 26 – July 1, 2023 (12:00 – 14:00 EST)
Total of hours: 12 hours

Course contents

1. **Introduction to Julia language and basics of programming** ***2 hours***
   - *a*) Introduction to Julia *30 min*
     1) Why Julia?
     2) Julia in computational chemistry
   - *b*) Installing and setting up the Julia environment *15 min*
   - *c*) Basic syntax and expressions *30 min*
     1) Variables, data types
     2) Operators, control structures
   - *d*) Functions and packages in Julia *30 min*
     1) Defining and calling functions
     2) Basic standard libraries
   - *e*) Hands-on coding practice *15 min*

2. **Data analysis in Julia** ***2 hours***
   - *a*) Data structures in Julia *30 min*
     1) Arrays, matrices, tuples, dictionaries
   - *b*) Introduction to DataFrames.jl package *30 min*
     1) Reading data from files
     2) Manipulating and summarizing data
   - *c*) Plotting data using Plots.jl *30 min*
   - *d*) Statistical analysis using the StatsBase.jl package *15 min*
   - *e*) Hands-on coding practice *15 min*

3. **Atomic simulations and quantum chemistry in Julia** ***2 hours***
   - *a*) Introduction to atomic simulations *15 min*
   - *b*) Molecular dynamics: basics and the role of Julia *30 min*
   - *c*) Overview of the JuLIP.jl and ASE.jl packages for atomic simulations *30 min*
   - *d*) Basics of quantum chemistry and Density Functional Theory *15 min*
   - *e*) Introduction to DFTK.jl package for electronic structure calculations *15 min*
   - *f*) Hands-on coding practice *15 min*

4. **Advanced topics in atomic simulations** ***2 hours***
   - *a*) *Monte Carlo* simulations: basics and implementation in Julia *30 min*
   - *b*) Quantum Monte Carlo with the QMC.jl package *30 min*
   - *c*) Machine learning potentials with the GaussianProcesses.jl package *30 min*
   - *d*) Introduction to the JuML.jl package for multi-scale modeling *15 min*
   - *e*) Hands-on coding practice *15 min*

5. **Data science for chemists** ***2 hours***
   - *a*) Application of machine learning in chemistry *15 min*
   - *b*) Introduction to ScikitLearn.jl for machine learning *30 min*
   - *c*) Clustering, PCA, and regression analysis *30 min*
   - *d*) Deep learning for chemistry with Flux.jl *30 min*
   - *e*) Hands-on coding practice *15 min*

6. **Research automation and high-performance computing** ***2 hours***
   - *a*) Overview of research automation *15 min*
   - *b*) scripting and pipeline development for automation *30 min*
   - *c*) Introduction for high-performance computing in Julia *15 min*
   - *d*) Parallel computing in Julia with the Distributed.jl package *30 min*
   - *e*) Best practices and next steps in Julia for computational chemists *15 min*
   - *f*) Hands-on coding practice and course wrap-up *15 min*