# QuDynamics: Julia package for solving Dynamical Equations in Quantum Mechanics

#### Amit

BITS-Pilani and Fudan University

Julia Users Meetup, University of Science and Technology of China

25-12-2015



What is Julia and Why?! Hello World! Julia

#### Introduction to Julia

Functions, Methods, Types Packaging in Julia

#### JuliaQuantum: QuBase, QuDynamics

QuBase and QuDynamics Defining a Quantum System Examples in QuDynamics

#### QuDynamics and FOSS

What is Git ?! Contributing to FOSS and QuDynamics





## What is Julia and Why ?!

▶ Julia is a high-level, high-performance programming language for technical computing.



QuDynamics and FOSS

- ▶ Julia is a high-level, high-performance programming language for technical computing.
- Julia is written in Julia (Base).



- ▶ Julia is a high-level, high-performance programming language for technical computing.
- Julia is written in Julia (Base).
- Performace as fast as compared to C (Every language has a tradeoff but Julia aims to be optimal for scientific computing).

- ▶ Julia is a high-level, high-performance programming language for technical computing.
- Julia is written in Julia (Base).
- Performace as fast as compared to C (Every language has a tradeoff but Julia aims to be optimal for scientific computing).
- ▶ Parallelization techniques and distributed computing come along with the base distribution.

•00000000

- ▶ Julia is a high-level, high-performance programming language for technical computing.
- Julia is written in Julia (Base).
- Performace as fast as compared to C (Every language has a tradeoff but Julia aims to be optimal for scientific computing).
- Parallelization techniques and distributed computing come along with the base distribution.
- Julia is FOSS allowing discussion of internals and design.



## Hello World! Julia



#### Hello World! Julia

Use either SageMathCloud (cloud.sagemath.com) (or) JuliaBox (juliabox.org).



#### Hello World! Julia

- Use either SageMathCloud (cloud.sagemath.com) (or) JuliaBox (juliabox.org).
- REPL Read Evaluate Print Loop



#### Hello World! Julia

- Use either SageMathCloud (cloud.sagemath.com) (or) JuliaBox (juliabox.org).
- REPL Read Evaluate Print Loop
- ▶ Hello World ! -> println("Hello World !")



QuDynamics: Julia package for solving Dynamical Equations in Quantum Mechanics

Functions



- Functions
- Structure which takes a tuple and returns a value



- Functions
- Structure which takes a tuple and returns a value
- Methods (OOP reference -> functional programming)

- Functions
- Structure which takes a tuple and returns a value
- Methods (OOP reference -> functional programming)
- One possible behavior for a function is called a method (Multiple Dispatch)



- Functions
- Structure which takes a tuple and returns a value
- ▶ Methods (OOP reference > functional programming)
- One possible behavior for a function is called a method (Multiple Dispatch)
- Types



- Functions
- Structure which takes a tuple and returns a value
- ▶ Methods (OOP reference − > functional programming)
- One possible behavior for a function is called a method (Multiple Dispatch)
- Types
- Examples !



# Packaging in Julia!



# Packaging in Julia!

► REPL *Pkg* usage



- ► REPL *Pkg* usage
- Using Pkg.add(), Pkg.clone(), Pkg.rm(), Pkg.installed(), Pkg.status()

#### QuBase & QuDynamics

### QuBase & QuDynamics

QuBase aims to provide all the basic machinery used in QM.



### QuBase & QuDynamics

- QuBase aims to provide all the basic machinery used in QM.
- QuDynamics uses the constructs of QuBase along with the Base machinery.



QuStateEvolution (alias QuPropagator) construct



- QuStateEvolution (alias QuPropagator) construct
- Hamiltonian, initial state, time steps, Methods



- QuStateEvolution (alias QuPropagator) construct
- Hamiltonian, initial state, time steps, Methods
- Methods: QuEuler, QuCrankNicolson, QuKrylov, QuODE45, QuODE78, QuODE23s, QuExpmV, QuExpokit, QuMCWF

- QuStateEvolution (alias QuPropagator) construct
- Hamiltonian, initial state, time steps, Methods
- Methods: QuEuler, QuCrankNicolson, QuKrylov, QuODE45, QuODE78, QuODE23s, QuExpmV, QuExpokit, QuMCWF
- ▶ System input include − > Schrodinger Eq. Liouville von Neumann Eq. Lindblad Master Eq.

- QuStateEvolution (alias QuPropagator) construct
- ► Hamiltonian, initial state, time steps, Methods
- Methods: QuEuler, QuCrankNicolson, QuKrylov, QuODE45. QuODE78, QuODE23s, QuExpmV, QuExpokit, QuMCWF
- ▶ System input include − > Schrodinger Eq. Liouville von Neumann Eq. Lindblad Master Eq.
- ▶ Configurations allowed! -> Operator matrix with state vector. Operator matrix with density matrix.

- QuStateEvolution (alias QuPropagator) construct
- ► Hamiltonian, initial state, time steps, Methods
- Methods: QuEuler, QuCrankNicolson, QuKrylov, QuODE45, QuODE78, QuODE23s, QuExpmV, QuExpokit, QuMCWF
- System input include -> Schrodinger Eq, Liouville von Neumann Eq, Lindblad Master Eq.
- ▶ Configurations allowed ! > Operator matrix with state vector, Operator matrix with density matrix.
- Other ways of specifying ! -> QuSchrodingerEq(pass the operator) Internally passing a operator matrix creates an equation.



- QuStateEvolution (alias QuPropagator) construct
- ► Hamiltonian, initial state, time steps, Methods
- Methods: QuEuler, QuCrankNicolson, QuKrylov, QuODE45, QuODE78, QuODE23s, QuExpmV, QuExpokit, QuMCWF
- ▶ System input include − > Schrodinger Eq. Liouville von Neumann Eq. Lindblad Master Eq.
- ▶ Configurations allowed! -> Operator matrix with state vector. Operator matrix with density matrix.
- ▶ Other ways of specifying ! -> QuSchrodingerEq(pass the operator) Internally passing a operator matrix creates an equation.
- Quantum Monte Carlo Wave Function Method (Test case) example)



### What is Git ?!

### What is Git ?!

▶ Git is a version control system.

#### What is Git ?!

- Git is a version control system.
- Clones, forks, branches ?!



000000000

- Git is a version control system.
- Clones, forks, branches ?!
- Push, pull, remotes!

000000000



QuDynamics is FOSS. (MIT license)



000000000

- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch



- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.

- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!

- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!
- Some of the WIP and future tasks can be found on the issue tracker

- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!
- Some of the WIP and future tasks can be found on the issue tracker
- ▶ Time dependency, QuTiP interface, Docs, QuBase independency, parallelization!



- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!
- ▶ Some of the WIP and future tasks can be found on the issue tracker
- ▶ Time dependency, QuTiP interface, Docs, QuBase independency, parallelization!
- To add more solvers refer to the Wiki page!



- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!
- ▶ Some of the WIP and future tasks can be found on the issue tracker
- ▶ Time dependency, QuTiP interface, Docs, QuBase independency, parallelization!
- ▶ To add more solvers refer to the Wiki page!
- More development notes on the news page of JuliaQuantum tagged as GSoC.



- QuDynamics is FOSS. (MIT license)
- Fork the repo, Clone locally, New branch
- Test locally, include the tests.
- Send in a PR (Pull Request) against the master!
- ▶ Some of the WIP and future tasks can be found on the issue tracker
- ▶ Time dependency, QuTiP interface, Docs, QuBase independency, parallelization!
- ▶ To add more solvers refer to the Wiki page!
- More development notes on the news page of JuliaQuantum tagged as GSoC.
- Example



#### Thank you



- Done as a part of Google Summer of Code 2015
- Mentored by Dr. Alexander Croy, Max Planck Institute for the Physics of Complex Systems, Germany.
- Repo : https://github.com/JuliaQuantum/QuDynamics.jl

