Advanced Topics from Scientific Computing
TU Berlin Winter 2024/25
Notebook 03
Jürgen Fuhrmann

These are the slides of a talk given at the 1st MaRDI workshop on Scientific Computing, October 2022

1st MaRDI Workshop on Scientific Computing

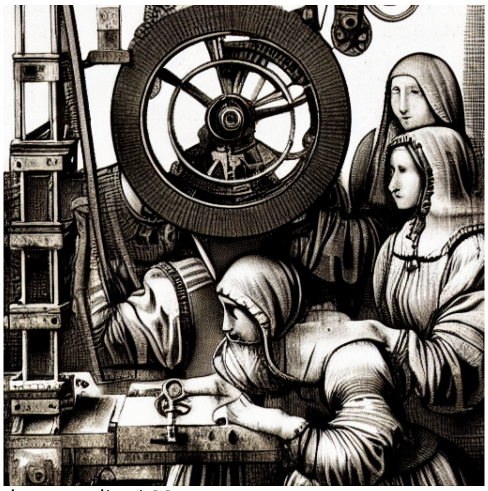
Reproducibility infrastructure of the Julia language

Jürgen Fuhrmann
WIAS Berlin

The Two Language Problem

... is at least a **three language problem**: you need to consider the **build system**, and at present we are talking about **CMake**...

- **Each project needs its own guru** to maintain the build system and to help to compile the code on new machines or to maintain docker containers
- Python APIs are easy to explain to general users, efficient algorithms are implemented in C/C++. **Python project codebases are intransparent for many of their users**
- **Containers are the new binaries**

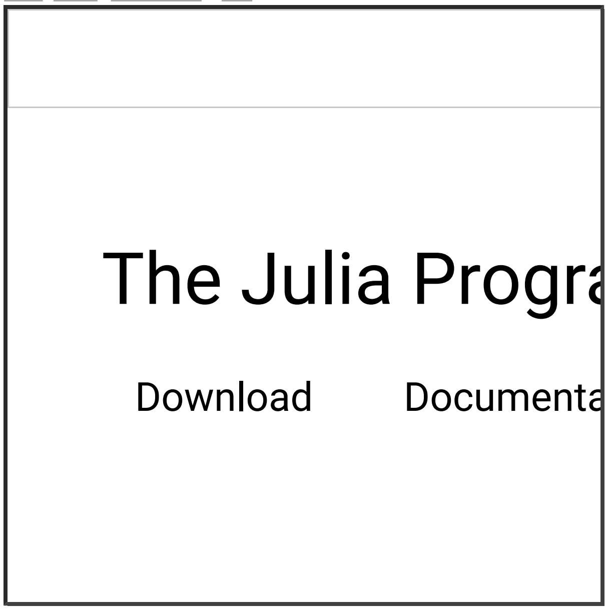

dreamstudio.ai CC01.0

We are in an **exponential boundary layer hitting a wall** regarding the complexity of build systems

Julia

- Syntax comparable to matlab, python/ numpy
- Just-ahead-of time compilation to native code ⇒ high potential for performance without need to vectorize or to call a computational kernel in another language
- Performant multi-dimensional arrays
- Comprehensive linear algebra
- Parallelization: SIMD, multithreading, distributed
- Interoperability with C, C++, python, R . . .
- Use of modern knowledge in language design
- Open source (MIT License)

https://julialang.org



The Julia Progra

Download Documenta

Packages

Packages extend Julia's core functionality. Each package is a git repository with standardized structure.

- **Package Registries** provide the infrastructure for finding package repositories via package names
- Default **General Registry**: ≈ 11500 open source packages (October 2024)
- Pkg.jl - the built-in **Package Manager** is part of the Julia standard library
- **Composability** of packages due to generic Julia source code (like C++ header only libs)

xkcd.com

```
#!/bin/bash

pip install "$1" &
easy_install "$1" &
brew install "$1" &
npm install "$1" &
yum install "$1" & dnf install "$1" &
docker run "$1" &
pkg install "$1" &
apt-get install "$1" &
sudo apt-get install "$1" &
steamcmd +app_update "$1" validate &
git clone https://github.com/"$1"/"$1" &
cd "$1";./configure;make;make install &
curl "$1" | bash &
```

Anatomy of a Julia package

Julia packages have a standardized structure

- Locally, each package is stored in a directory named e.g. `MyPack` for package `MyPack.jl`.
- Structure of a package directory:
  - `MyPack/src`: subdirectory for package source code
    - `MyPack/src/MyPack.jl`: code defining a module `MyPack`
    - Further Julia sources included by `MyPack.jl`
  - `MyPack/test`: code for unit testing
  - `MyPack/docs`: markdown sources + code for documentation
  - LICENSE: (open source) license
  - Project.toml: Metadata

```
PcZ48
├─ .github
│  ⋮
│
├─ .gitignore
├─ LICENSE.md
├─ Project.toml
├─ README.md
├─ benchmarks
│  ⋮
│
├─ docs
│  ⋮
│
├─ ext
│  ⋮
│
├─ src
│  ⋮
│
└─ test
   ⋮
```

Package metadata

Contents of `Project.toml` for the ForwardDiff.jl package

```
name = "ForwardDiff"
uuid = "f6369f11-7733-5829-9624-2563aa707210"
version = "0.10.36"

[deps]
CommonSubexpressions = "bbf7d656-a473-5ed7-a52c-81e309532950"
DiffResults = "163ba53b-c6d8-5494-b064-1a9d43ac40c5"
DiffRules = "b552c78f-8df3-52c6-915a-8e097449b14b"
LinearAlgebra = "37e2e46d-f89d-539d-b4ee-838fcccc9c8e"
LogExpFunctions = "2ab3a3ac-af41-5b50-aa03-7779005ae688"
NaNMath = "77ba4419-2d1f-58cd-9bb1-8ffee604a2e3"
Preferences = "21216c6a-2e73-6563-6e65-726566657250"
Printf = "de0858da-6303-5e67-8744-51eddeeeb8d7"
Random = "9a3f8284-a2c9-5f02-9a11-845980a1fd5c"
SpecialFunctions = "276daf66-3868-5448-9aa4-cd146d93841b"
StaticArrays = "90137ffa-7385-5640-81b9-e52037218182"

[compat]
Calculus = "0.2, 0.3, 0.4, 0.5"
CommonSubexpressions = "0.3"
DiffResults = "0.0.1, 0.0.2, 0.0.3, 0.0.4, 1.0.1"
DiffRules = "1.4.0"
DiffTests = "0.0.1, 0.1"
LogExpFunctions = "0.3"
NaNMath = "0.2.2, 0.3, 1"
Preferences = "1"
SpecialFunctions = "0.8, 0.9, 0.10, 1.0, 2"
StaticArrays = "0.8.3, 0.9, 0.10, 0.11, 0.12, 1.0"
julia = "1"

[extensions]
ForwardDiffStaticArraysExt = "StaticArrays"
```

Package metadata

Contents of `Project.toml`

- Package name
- UUID to identify package, name is secondary
  - ⇒ manage different packages with the same name
- Version according to Semantic Versioning
- `[deps]` section: list of package dependecies with UUIDs
- `[compat]` section: version compatibility bounds for dependencies and julia
- Further info: author, additional packages for testing . . .

dreamstudio.ai CC01.0

Adding a package

```
julia> Pkg.add("MyPkg")
```

1. Package name and UUID are looked up in a **registry**
2. Package git repo URL read from registry (nowadays packages are cached and served from a package server by default)
3. Calculation of version compatibility for package and dependencies
4. Code of package and dependencies downloaded to `~/.julia/packages/`
5. Package and dependencies recorded in current active **environment**

dreamstudio.ai CC01.0

After adding a package, `using MyPkg` allows to use the package content in a Julia session or project source.

Registries

A **registry** is a directory collecting metadata of packages for look-up

- Default: https://github.com/JuliaRegistries/General
  - Like blockchain: no deletions, continued forever
  - Packages must be open source
  - Automated heuristic decision process for new packages to be registered
- Local copy kept up-to-date for each Julia installation
- Multiple (e.g. institutional) registries are possible

dreamstudio.ai CC01.0

Environments

Environment: directory with `Project.toml` and `Manifest.toml`

- `Project.toml`: name + UUIDs of all packages added
- `Manifest.toml`: name + UUID + version + git-hash of package *and all of its depedencies and their dependencies*
- Each project can have its own environment
  - `$ julia`: activate default environment for julia version, e.g. `~/.julia/environments/v1.7`
  - `$ julia --project=@xyz`: activate environment in `~/.julia/environments/xyz`
  - `$ julia --project=dir` and `julia> Pkg.activate("dir")` activate environment in directory `dir`

dreamstudio.ai CC01.0

Further features & details

- Consistent package updates
- Package garbage collection
- Access to older revisions and git branches
- Standardized test environment for Julia packages. Julia core developers can test new julia versions with the registered packages to find out regressions
- **Artifacts**: `Artifacts.toml` records BLOBS available at given URL + content hash to be installed along with a project/package without the need to have them in git
- **Binary (jll) packages**: pre-built, cross compiled libraries for all relevant architectures managed as Artifacts allow to use libraries implemented in other languages in a simple an reliable way
  - See the Yggdrasil repository for the build scripts for all registered jlls

Reproducible projects

Transferring `Project.toml` and `Manifest.toml` allows to reproduce the exact package composition of a project

- **Alice**, working on Linux, creates a project using Julia and **a number of Julia packages**. She develops the code in a directory which is activated as a Julia environment. She sets up a git repository containing source code, documentation and both `Project.toml` and `Manifest.toml` files.
- **Bob**, working on windows with the same Julia version, checks out the code from the repo. A call to `Pkg.instantiate()` **installs all packages** in the exact combination of versions as Alice had them on her computer.

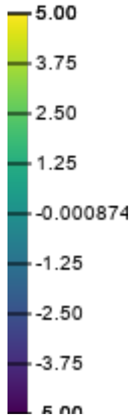
dreamstudio.ai CC01.0

Reproducible Notebooks: Pluto.jl

Browser based notebooks implemented in Julia and Javascript

- **Easy installation**: installed as a single Julia package on Linux, MacOS, Windows
- **Reactive**: cell results are automatically recalculated
- **Version controllable**: no computational results in the notebook
- **Reproducible**: notebooks contain their own environment
- Efficient interaction with HTML+Javascript
- Created by Fons van der Plas & his friends

PlutoVista.jl+vtk.js+webgl: 132651 nodes



```julia
f(x,y,z)=sin(x)*cos(3y)*z;
```

More Pluto.jl Benefits

- **Clara** teaches a Julia based course in scientific computing. She prepares the **course material as Pluto notebooks**. After installation with simple instructions, **students run them** on their computers. The package environment automatically installs all packages necessary for a notebook. HTML and PDF previews available as well.
- **Students** prepare their **exam projects as Pluto notebooks**. Clara can receive their work and run it on her computer.
- MIT (Computational Thinking), TU Berlin (Scientific Computing) . . .

Download Julia and install it according to the procedure on you particular operating system. Invoke Julia and issue the following commands:

```
using Pkg
Pkg.add("Pluto")
using Pluto
Pluto.run()
```

A menu will show up in the browser which allows to start the notebooks downloaded from the course homepage.

Further infrastructure

- DrWatson.jl manages code and computational results in a Julia project repository
    - Automatic generation of data file names from simulation parameters
- Documenter.jl: documentation
    - from docstrings in package sources
- Visual Studio Code integration
- Jupyter notebook support
- Integration with quarto for reproducible publications

Some Issues

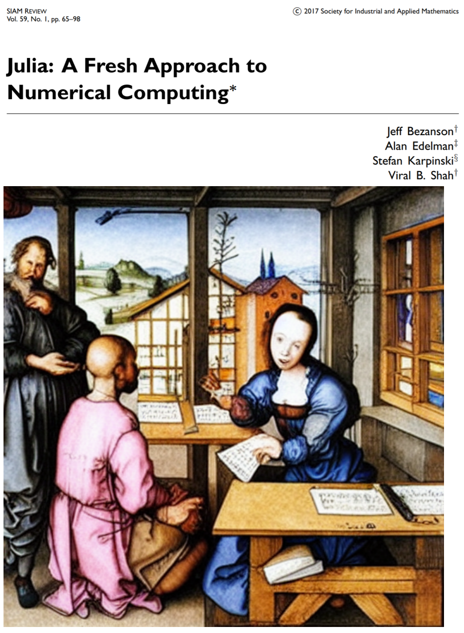
- Package loading and `using` latency due to JIT precompilation aka "Time to first plot"
  - Currently, the Julia community undertakes dedicated successful efforts towards fixing this problem
- Missing formal interface descriptions
  - Julia alternative to C++20 concepts ? Traits ?
  - Bottom up design process, fear to lose opportunities due to too rigid formalizations
- Resources for keeping infrastructure running
  - Many volunteers are involved at central points
  - Competitivity depends on package contributions
  - Server infrastructure costs

dreamstudio.ai CC01.0

Conclusions

Julia provides as well a **fresh approach to reproducibility**, learning from the experiences of of `conda`, `npm` etc.

- Package management is part of the standard Julia workflow, available without further installation
- Transparent package and project source code without the need to know two languages or handling of build systems
- Introductions to Julia at an early stage should explain working with environments etc.
- Can we contribute to Julia and its infrastructure from the NFDI context ? (Same question for other open source ecosystems . . .)


SIAM REVIEW
Vol. 59, No. 1, pp. 65–98

© 2017 Society for Industrial and Applied Mathematics

Julia: A Fresh Approach to Numerical Computing*

Jeff Bezanson†
Alan Edelman‡
Stefan Karpinski§
Viral B. Shah†