# Scientific Computing With Rust

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Overview

Expressing Science with Software

Current Research Directions

Maturin Demo of Python+Rust Project

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### Team and Research Focus

#### Research Focus:

- Numerical Analysis & Scientific Computing
- 2. PDEs: Acoustics, Electromagnetics, Electrostatics
- High-Performance Computing and Software Engineering



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# My Research

# 'Science with Computers and Maths'

- 1. High Performance Computing
- 2. Heterogenous Computing
- 3. Software Engineering
- 4. Problems in Physics and Engineering



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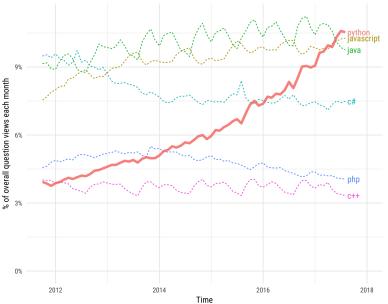
# Expressing Scientific Problems With Software

There is no 'best' language for expressing scientific problems with software.

Though Python has emerged as a defacto standard amongst scientists and engineers for a broad spectrum of problems.

#### **Growth of major programming languages**

Based on Stack Overflow question views in World Bank high-income countries



# The Two Language Problem

- Languages suited for human needs, are less efficient for computers to run.
- 2. Languages easy for computers to run efficiently, are correspondingly less easy for humans to use!

# Why Rust?

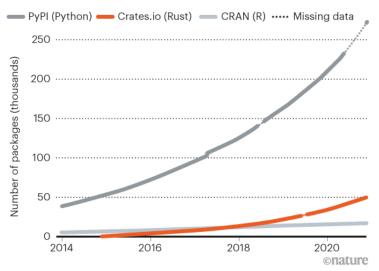
Don't many of the 'two language' problems still exist?

#### Pros of Rust:

- 1. Cargo is awesome!
- 2. Rust is Fast
- 3. Foreign language interfaces are easy
- 4. Easy to learn (harder to master)
- 5. Traits
- 6. Borrow Checker

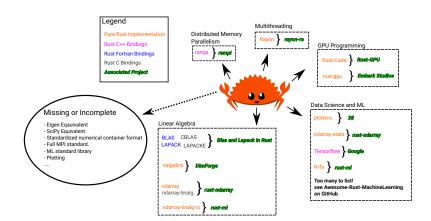
### **RUST RISING**

The Rust packages repository crates.io has grown sharply since 2016, mirroring the rapid uptake of the language.



https://www.nature.com/articles/d41586-020-03382-2

# State of Scientific Computing in Rust



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## A Splash of Differential Equations

What is an Ordinary Differential Equation?

Imposition of a relationship between functions of a independent single variable and its derivatives.

e.g. Newton's Second Law of Motion (in 1 Dimension)

$$m\frac{d^2x}{dt^2} = F(x(t)) \tag{1}$$

# A Splash of Differential Equations

What is a Partial Differential Equation?

Imposition of a relationship between functions of a multiple independent variables and their derivatives.

e.g. The Heat Equation (in 3D Cartesian Coordinates,

$$\Delta = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

$$\frac{du}{dt} = \Delta u \tag{2}$$

Where u(x, y, z, t).

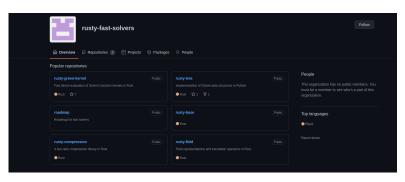
### **BEM**

# Problems with BEM

# **FMM**

### Fast Direct Solvers

### Rusty Fast Solvers Project



https://github.com/rusty-fast-solvers

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