JuliaHub

Accelerating Modeling and Simulation with Scientific Machine Learning in Julia

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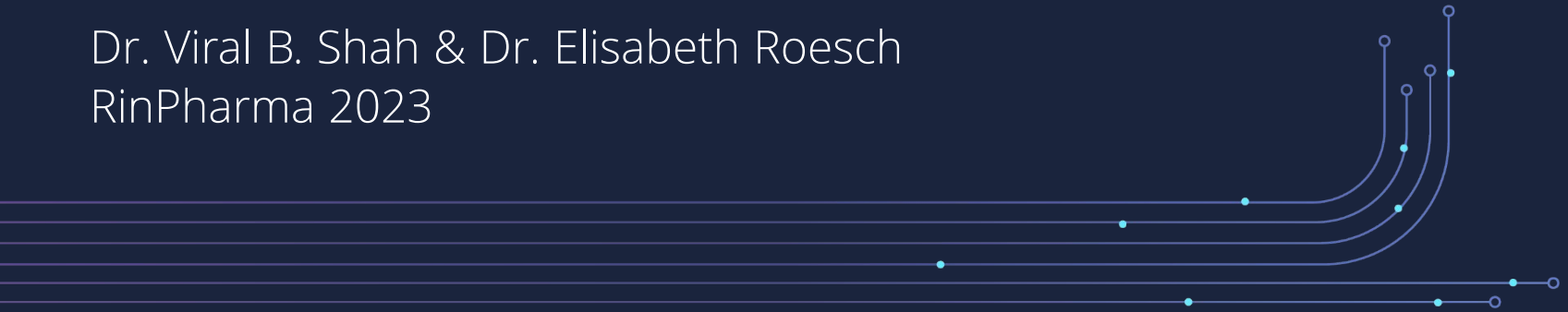
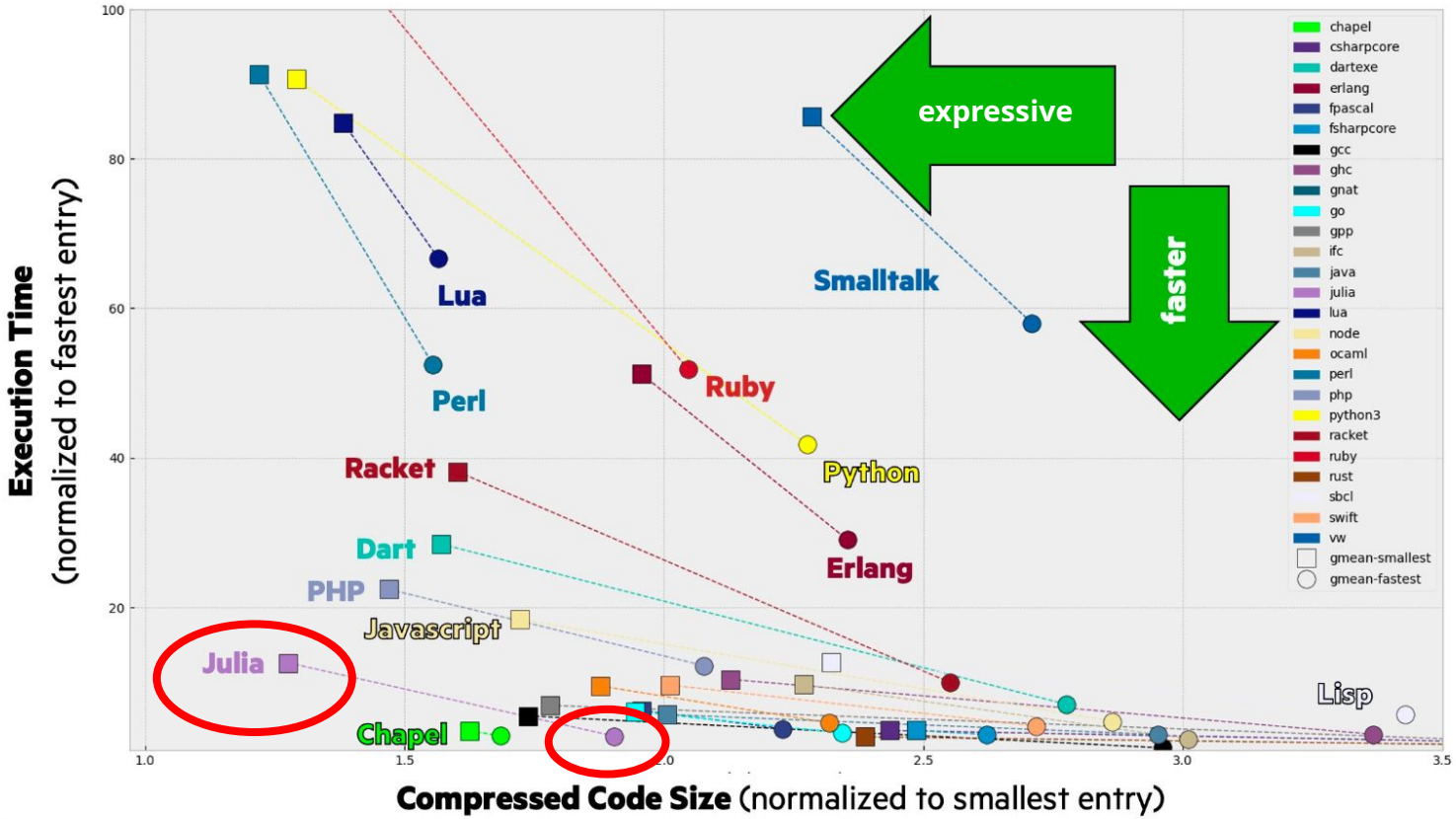
RinPharma 2023

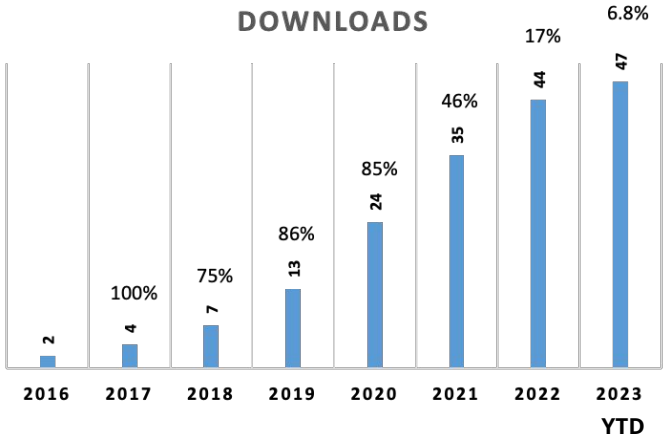


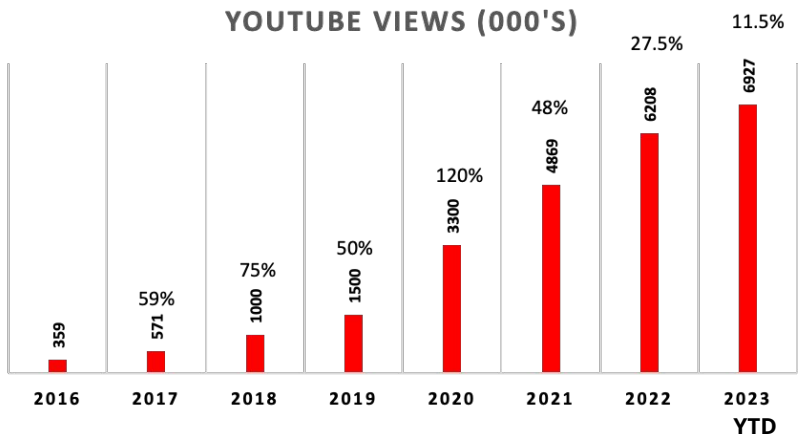
October 25, 2023

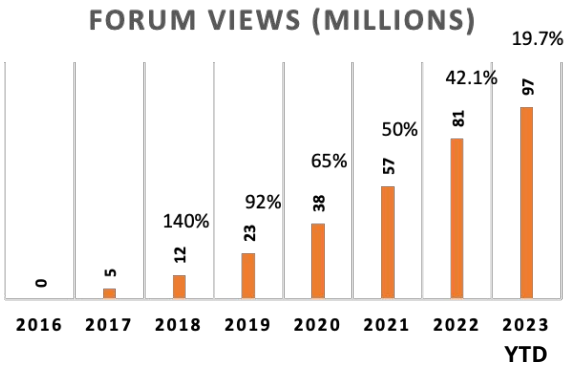
Julia is a high-level language that solves the two language problem

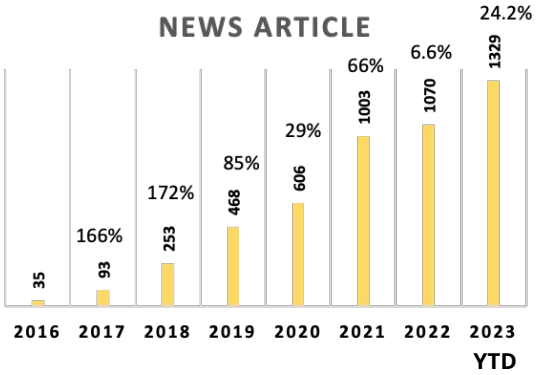


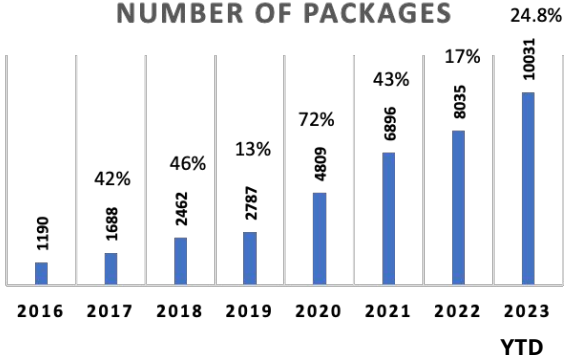
The Julia Community Is Growing





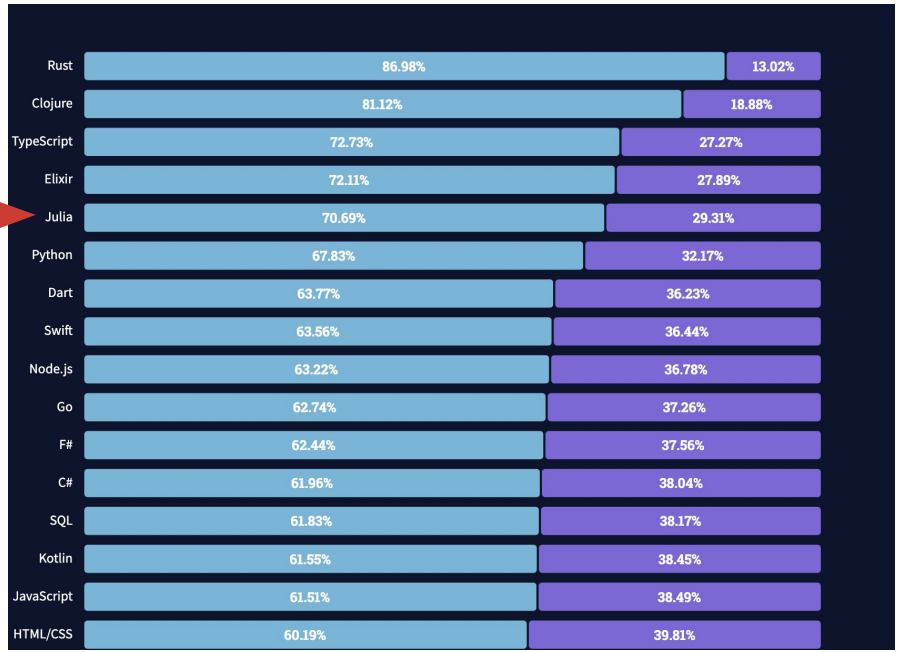




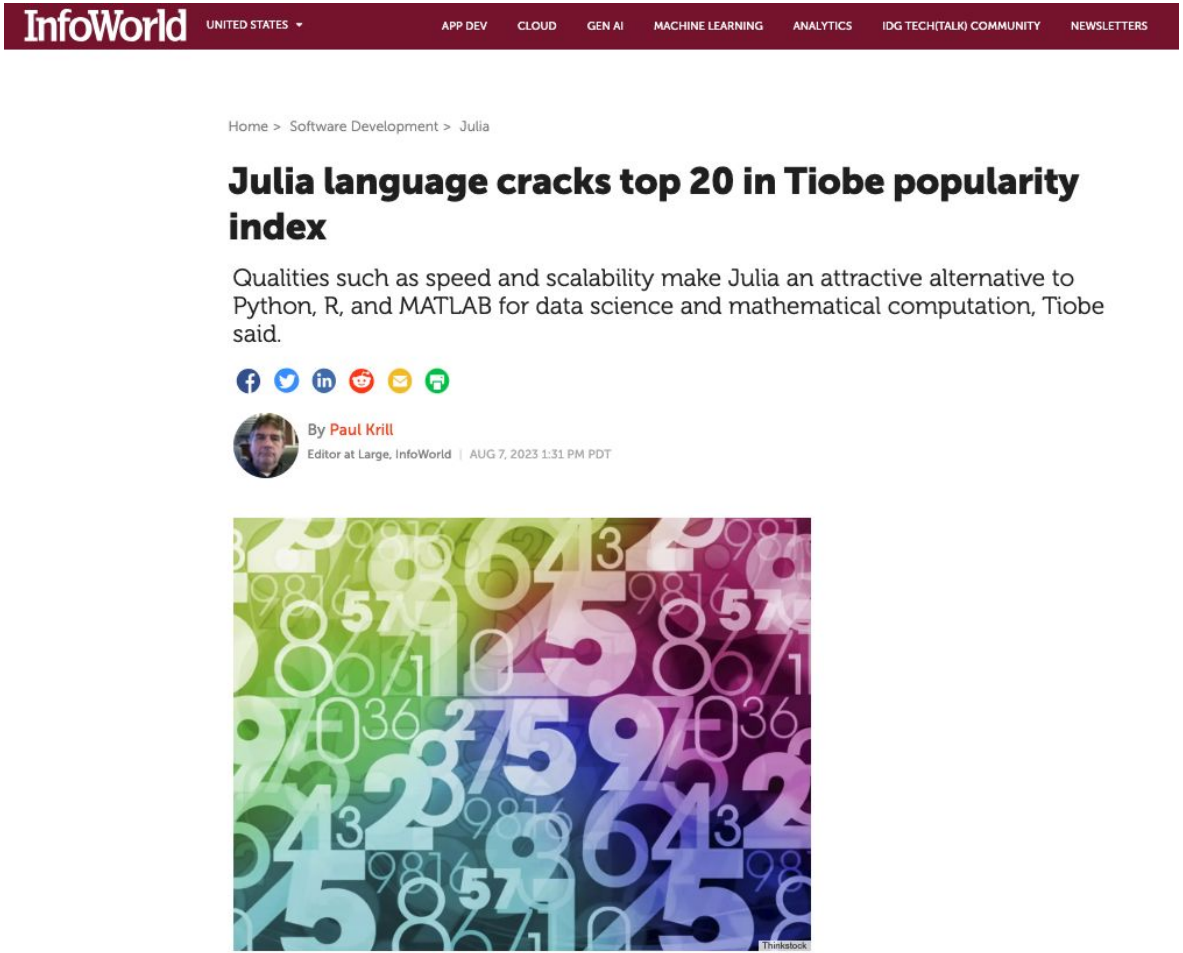


Julia: The Next Generation Technical Computing Language

- Purpose built from the ground up for technical computing
- Solves the “Two Language Problem”
- Vibrant and growing ecosystem
- 5th most loved programming language according to StackOverflow 2022!



More loved that Python (#6), R (#28) and MATLAB (#36)



[Julia made it to the Tiobe Top 20 in August 2023]

While the index is noisy, the trends are real

Starting at #47 in 2017, Julia made it to Top 20 in 2023.

Growing adoption in the pharma community

- JuliaCon talks:
  - Tidier.jl: Bringing the TidyVerse to Julia (U Mich)
  - Working with DataFrames.jl in Julia (Workshop)
  - Modeling and Simulation to Guide Dose Selection (Moderna)
  - Julia and SciML for QSP Modeling (Sanofi)
  - QSP Model for Pulmonary Arterial Hypertension (United Therapeutics)
  - UDEs for parameter estimation in Systems Biology (Univ. of Bonn)
  - BioMakie.jl - Plotting and Interface Tools for Biology (Iowa State Univ)
  - Exploring the State of Machine Learning for Biological Data (UT Dallas)
  - And many more…

Pumas Suite

Pumas

DeepPumas

PumasCP

PumasQSP

Pumas Suite USP

Accepted by Global Regulatory Agencies | Preferred by High Performance Teams

Scientists

- Developed by Users
- Best Minds in the Field
- **White Glove Service**
- Largest Development Team in Industry

Robust Platform

- Partnered with Inventors of Julia Language
- Vertically Aligned
- Engineered for Seamless Integration
- **Complete Programming Language**

Innovation

- **One Stop Shop**
- Adopting Latest Technology Promptly
- Pioneering New Methodologies
- Revamping MIDD Workflow
- Collaboratively drive innovation

Optimized for Performance

- Pumas Suite is Cloud-First Technology
- On-Demand Scalability
- Fully Validated
- **Designed for Collaboration**

The Pumas Interface

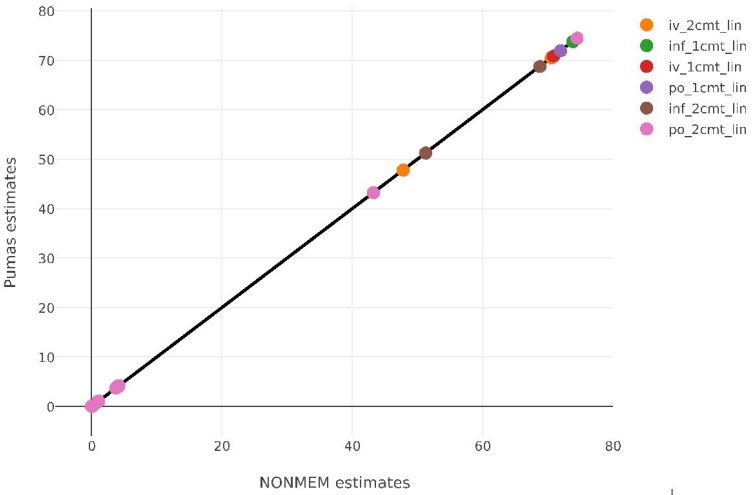
- @model macro defines a PumasModel
- Integrates with regular Julia functions
- Core integration with NCA routines
- Core integration with Distributions.jl

```
pk_1cmp = @model begin
  @param begin
    "Clearance (L/hr)"
    tvcl ∈ RealDomain(lower = 0, init = 3.2)
    "Volume (L)"
    tvv  ∈ RealDomain(lower = 0, init = 16.4)
    "Absorption rate constant (h^-1)"
    tvka ∈ RealDomain(lower = 0, init = 3.8)
    """
    - IIV CL
    - IIV V
    - IIV Ka
    """
    Ω    ∈ PDiagDomain(init = [0.04,0.04,0.04])
    "Proportional RUV"
    σₚ  ∈ RealDomain(lower = 0.0001, init = 0.2)
  end

  @random begin
    η ~ MvNormal(Ω)
  end

  @covariates DOSE

  @pre begin
    CL = tvcl * exp(η[1])
    Vc = tvv * exp(η[2])
    Ka = tvka * exp(η[3])
  end

  @dynamics Depots1Central1

  @derived begin
    cp := @. Central/Vc
    "Plasma DrugX Concentration (ng/mL)"
    dv ~ @. Normal(cp, cp*σₚ)
  end
end
```

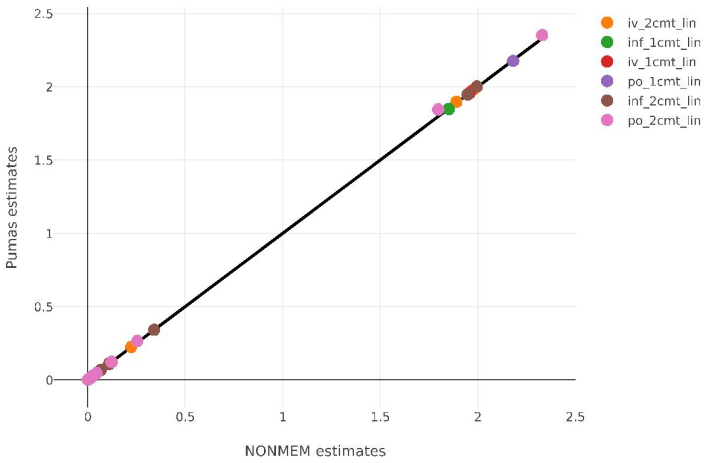
Backup slides

Accurate - Match NONMEM results

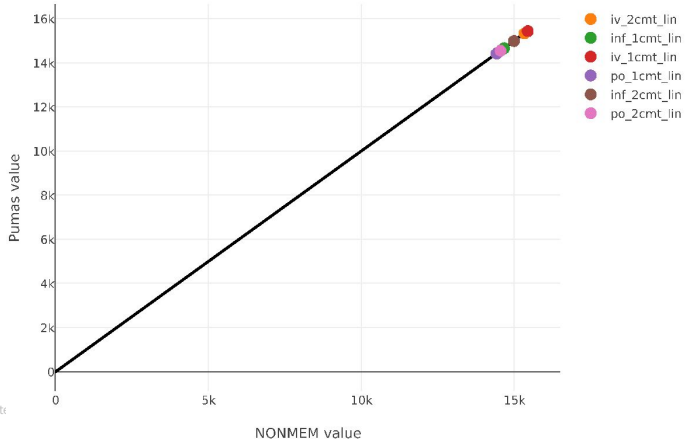
FOCEI parameter estimate comparisons using Serial - 1 thread



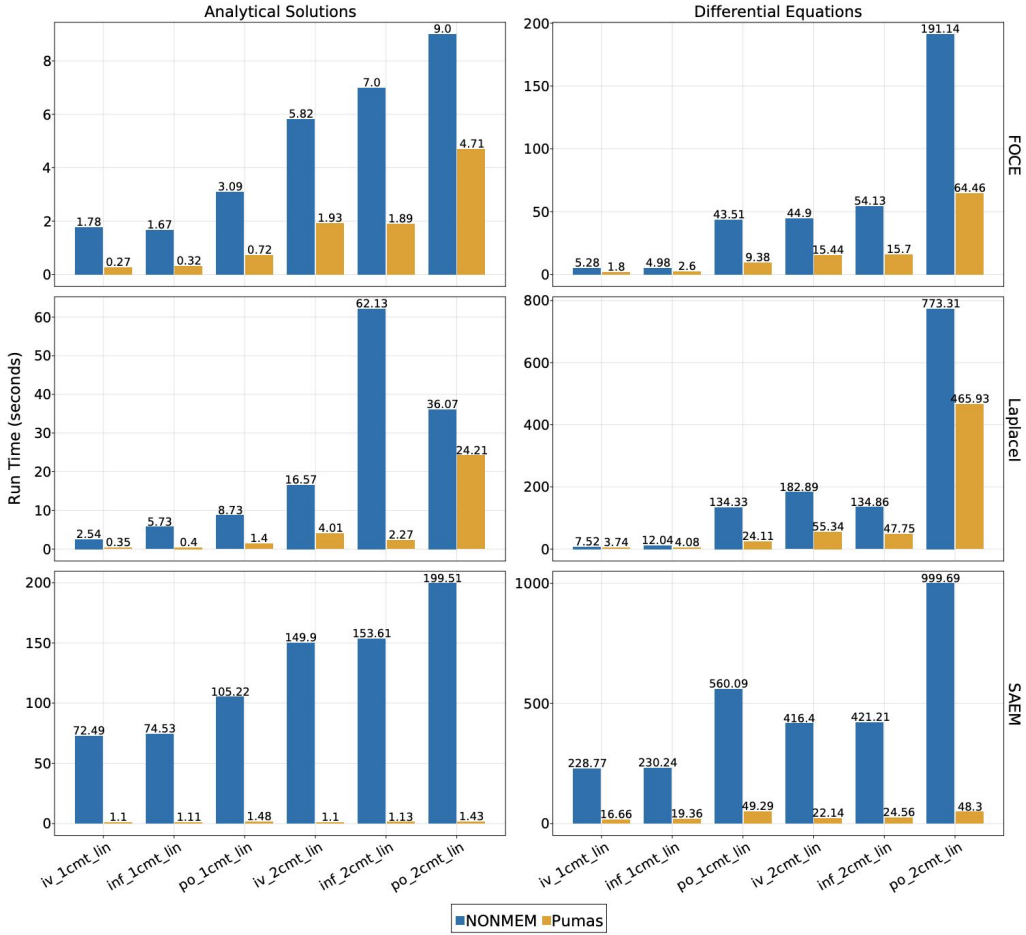
FOCEI standard error estimate comparisons using Serial - 1 thread



FOCEI -2LL comparison using Serial - 1 thread



Fast - across the board



Roadmap for Pumas Suite