

# Developing an RSE Workforce for Accelerating Computational, Data, and AI Applications



Democratizing Access to Research  
Software Engineering

SCIPe award 2417814

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Democratizing Access to  
Research Software  
Engineering

UNIVERSITY OF  
DELAWARE



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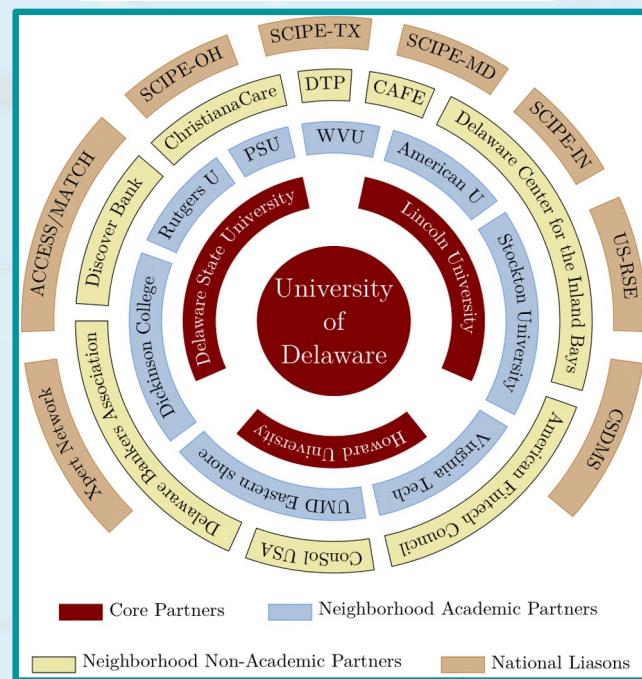
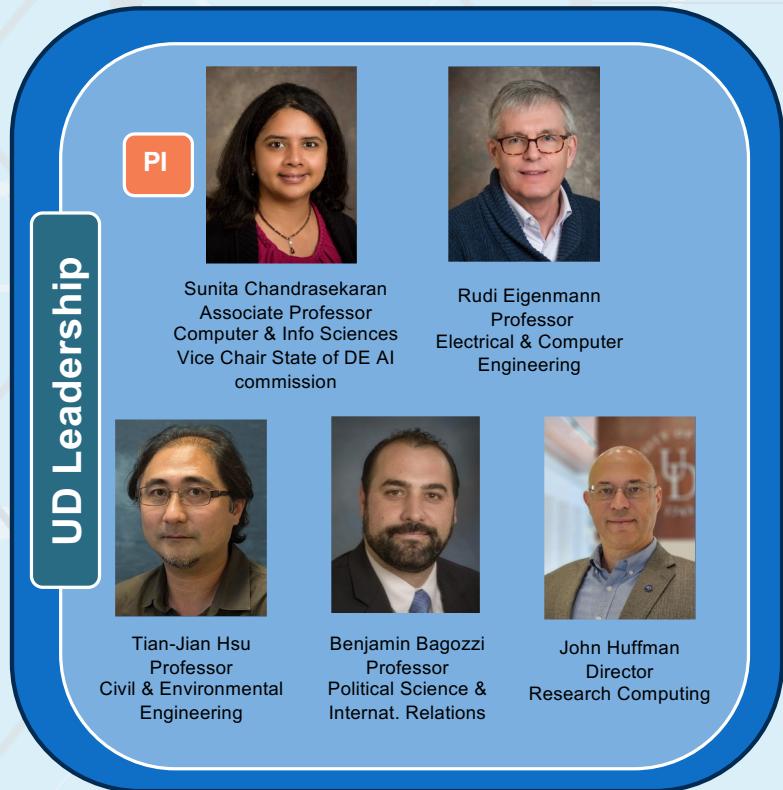


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# Who is Involved ?



Partners



# DARSE – Democratizing Access to Research Software Engineering

How

- Team of RSEs
- Educational pipeline



Why team of RSEs ?

- Expressed need by UDel faculty
- XSEDE/ECSS MVP
- Long-term mission to build infrastructure for computational/data/AI science



Why educational pipeline ?

- Not enough RSEs
- Understanding RSE role



# How Do You Organize a Team of Research Software Engineers ?

## Who?

- Hired professionals
- Student RSEs
- Link to similar roles at partner sites



Synergizing our RSEs within similar roles at the IT department and individual groups.

## Selecting Domain Projects?

- Advertising the service
- Selection criteria:
  - Science quality
  - Enabled new science



## Model of collaborative assistance

- 1-12 months typical

## Financial model

- 50/50 internal/external \$\$
- RSEs budgeted on research grants



## Another Important goal

- Developing best practices

# Creating the Next Generation of RSEs – Educational Pipeline



Individual courses

Certificates

Concentrations and full curricula



Teaching bandwidth

- Look for RSE-relevant existing courses
- Engage RSEs in teaching

# Understanding the RSE Role - RSE Professionalization

What is in the "R" in RSE ?

Differences from software engineering?

Examples

- Understanding domain sciences
- Understanding the academic environment
- Collaborative assistance  
(of rel. short duration)



HR challenge

- RSE job description includes both service and science
- RSE is not an IT department job !



We are not alone in this

- XSEDE/ECSS
- ACCESS, NAIRR
- CaRCC
- US-RSE
- Virtual Residency

# DARSE Project Status and What's Next ?

- One year into the project
- 2 Full-time RSEs newly hired
- Many proposed research projects, evaluated and selected
- Student RSEs engaged and working on projects as well
  - Several student volunteers from Master's in Data Science program
- Initial RSE course to be offered in Spring 2026
- Workshops in mid-Atlantic area



# The Atom Project – CSSI award 2209639

- PI: Marianna Safronova
- A portal for sharing data about atoms/ions with the community
- [udel.edu/atom](http://udel.edu/atom)

The screenshot shows the homepage of the Atom Project. At the top, there is a navigation bar with the University of Delaware logo, followed by links for Home, Elements (with a dropdown), Our Team, About (with a dropdown), Source Code, and several green buttons for Video Tutorial, Help, Feedback, and Citation Info. Below the navigation bar is a header with the text "Portal for High-Precision Atomic Data and Computation" and a small atomic model icon. A call-to-action text "Click on an element to display its properties" is centered. Below this, there are two grids of element cards. The left grid contains: Li, Be<sup>+</sup>, Na; Mg, Mg<sup>+</sup>, K; Ca, Ca<sup>+</sup>, Rb; Sr, Sr<sup>+</sup>, Cs; and Ba<sup>+</sup>, Fr, Ra<sup>+</sup>. The right grid contains: Cs<sup>6+</sup>, Ba<sup>7+</sup>, Ce<sup>9+</sup>; Pr<sup>10+</sup>, Nd<sup>11+</sup>, Nd<sup>12+</sup>; Nd<sup>13+</sup>, Sm<sup>13+</sup>, Sm<sup>14+</sup>; Sm<sup>15+</sup>, Eu<sup>14+</sup>, Cf<sup>15+</sup>; and Cf<sup>17+</sup>.



# Atom Portal – Data Example: Matrix Elements for State $2s_{1/2}$

The screenshot shows the Atom Portal interface for Lithium (Li). The top navigation bar includes links for Home, Elements, Our Team, About, and Source Code. Below the navigation is a menu bar with options: Video Tutorial, Help, Units, Feedback, Citation Info, Matrix elements (selected), Transition rates, Polarizabilities, Energies, Hyperfine constants, Nuclear data, and ASD.

The main content area displays a table of matrix elements for the  $2s_{1/2}$  state. The table has columns for Transition, Wavelength (nm), and Matrix element (a.u.). The transitions listed are from  $2s_{1/2}$  to various other states:  $2p_{1/2}$ ,  $2p_{3/2}$ ,  $3p_{1/2}$ ,  $3p_{3/2}$ ,  $3d_{3/2}$ ,  $3d_{5/2}$ ,  $4s_{1/2}$ ,  $4p_{1/2}$ ,  $4p_{3/2}$ ,  $4d_{3/2}$ ,  $4d_{5/2}$ ,  $4f_{5/2}$ ,  $4f_{7/2}$ , and  $5s_{1/2}$ . The matrix elements are numerical values with error bars, such as 3.3170(4) and 4.6907(6).

Transition	Wavelength (nm)	Matrix element (a.u.)
$2s_{1/2} \rightarrow 2p_{1/2}$	670.976(6)	3.3170(4) <a href="#">Ref</a>
$2s_{1/2} \rightarrow 2p_{3/2}$	670.961(6)	4.6907(6) <a href="#">Ref</a>
$2s_{1/2} \rightarrow 3p_{1/2}$	323.359(1)	0.18293(17)
$2s_{1/2} \rightarrow 3p_{3/2}$	323.359(1)	0.25870(30)
$2s_{1/2} \rightarrow 4p_{1/2}$	274.201(1)	0.160101(80)
$2s_{1/2} \rightarrow 4p_{3/2}$	274.201(1)	0.22642(13)
$2s_{1/2} \rightarrow 5p_{1/2}$	256.3080(9)	0.119749(60)
$2s_{1/2} \rightarrow 5p_{3/2}$	256.3080(9)	0.169352(85)
$2s_{1/2} \rightarrow 6p_{1/2}$	247.5809(9)	0.09251(30)
$2s_{1/2} \rightarrow 6p_{3/2}$	247.5809(9)	0.13083(43)

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# Atom Portal – Data Example: Polarizability Graphs



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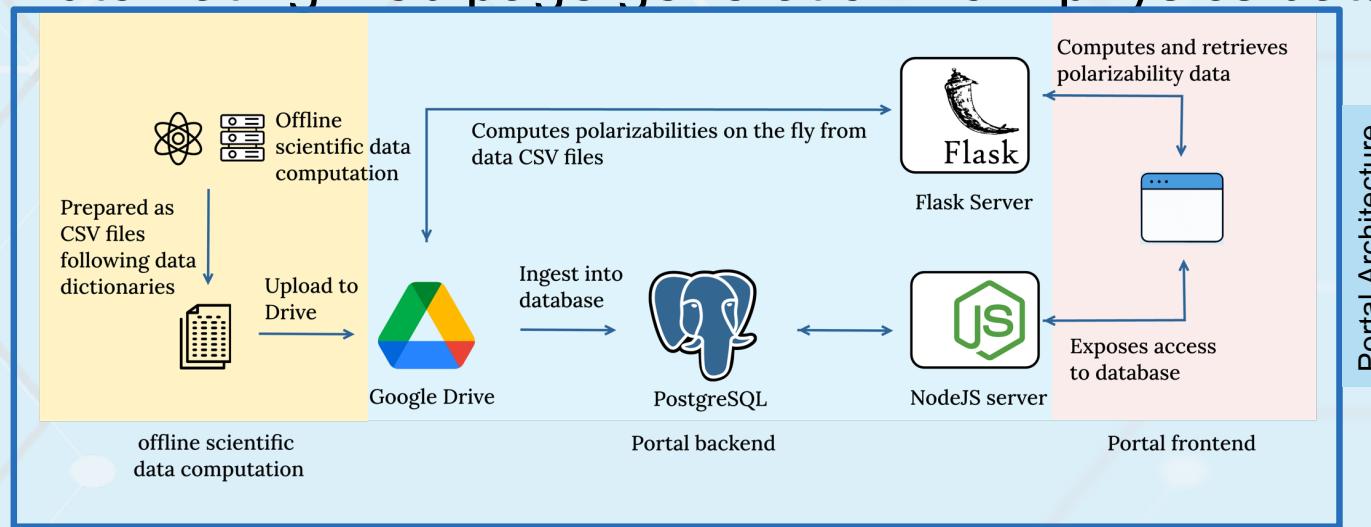


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# Atom Portal: Challenges on the Computer Science Side

- Automating web page generation from physics data



- Collaboration with physicists

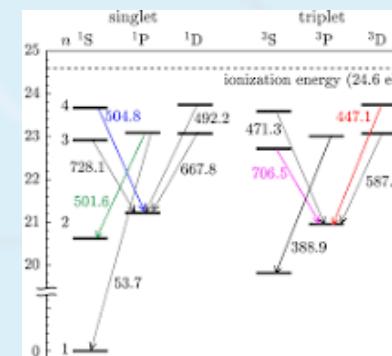
# Atom Portal Project: Status and What's Next?

Portal Version 3 released in June 2025:

- 28 atoms/ions
- Energies, transition matrix elements, transition rates, radiative lifetimes, branching ratios, polarizabilities, hyperfine constants

Next

- Include additional atoms/ions
- Grotrian diagrams
- Extract experimental data from tables in published papers



# Role of Artificial Intelligence in SCIPE, CSSI, and Other Projects

AI for DARSE and Atom projects



For other projects:

- ICICLE NSF AI Institute The logo for ICICLE (DEMOCRATIZING AI) features a stylized brain icon composed of interconnected nodes and lines, with the word "ICICLE" in white capital letters above the text "DEMOCRATIZING AI".
- UD AI Center of Excellence
- XAI - out of distribution data - e.g. extreme weather events
- First State AI Institute The logo for the First State AI Institute features the word "NEW" in a large, white, stylized font with a red shadow effect.

# Thanks for Listening !

Any Questions



Contact us. [darse-scope@udel.edu](mailto:darse-scope@udel.edu)