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

Democratizing Access to Research Software Engineering

SCIPE award 2417814

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Who is Involved ?

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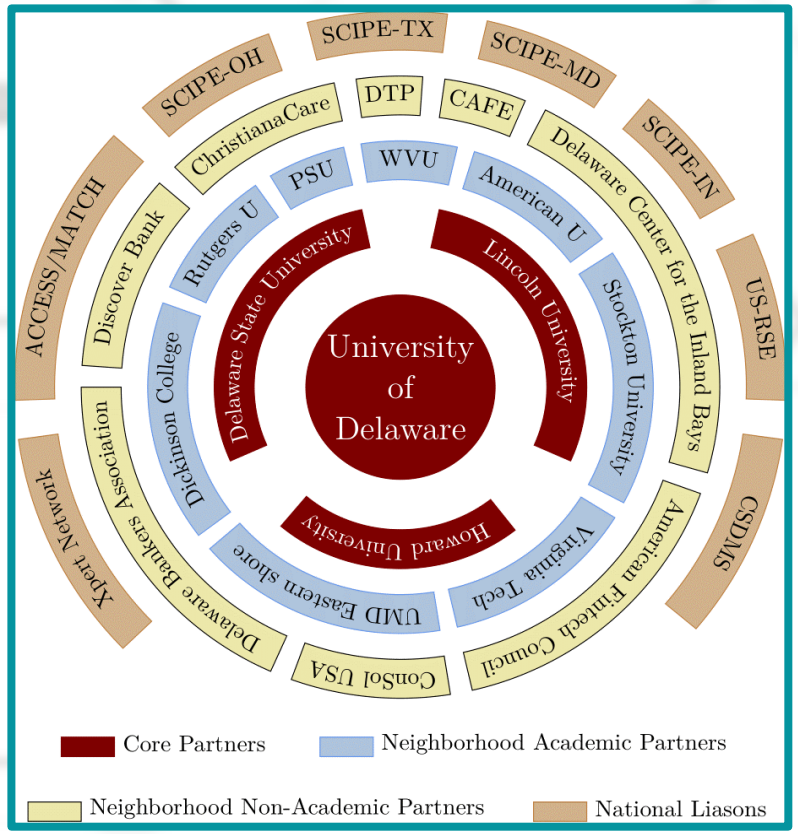
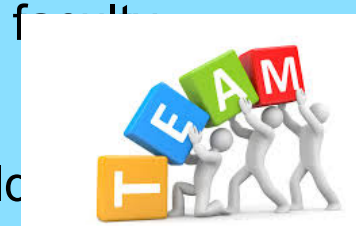


DARSE – Democratizing Access to Research Software Engineering

How
- Team of RSEs
- Educational pipeline

Why team of RSEs ?
- Expressed need by UDel f
- XSEDE/ECSS MVP
- Long-term mission to build
for computational/data/AI



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 Importa

- 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

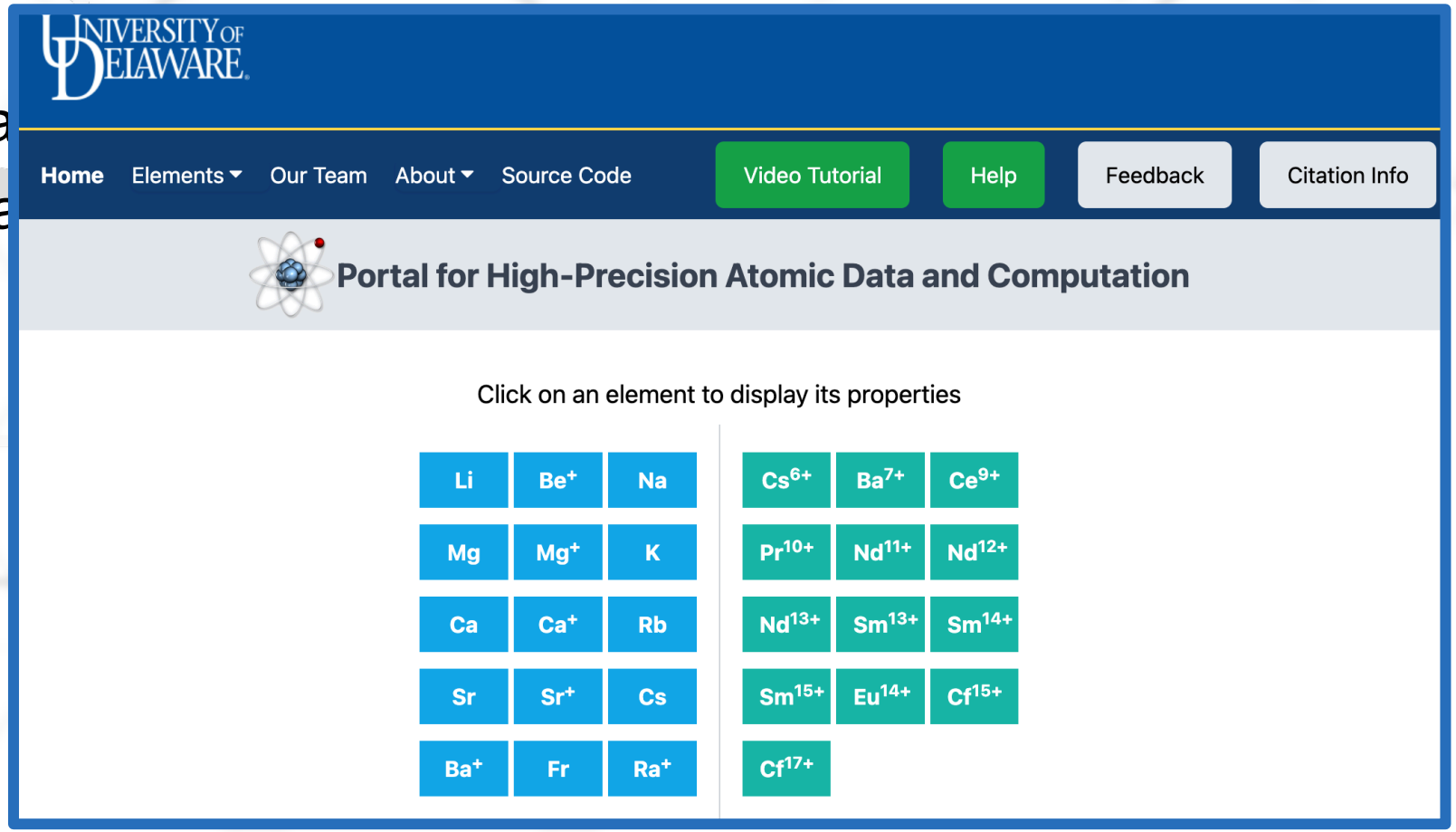
- XSEDE/ECSS
- ACCESS, NAIRR
- CaRCC
- US-RSE
- Virtual Residency

DARSE Project Status and What's Next ?

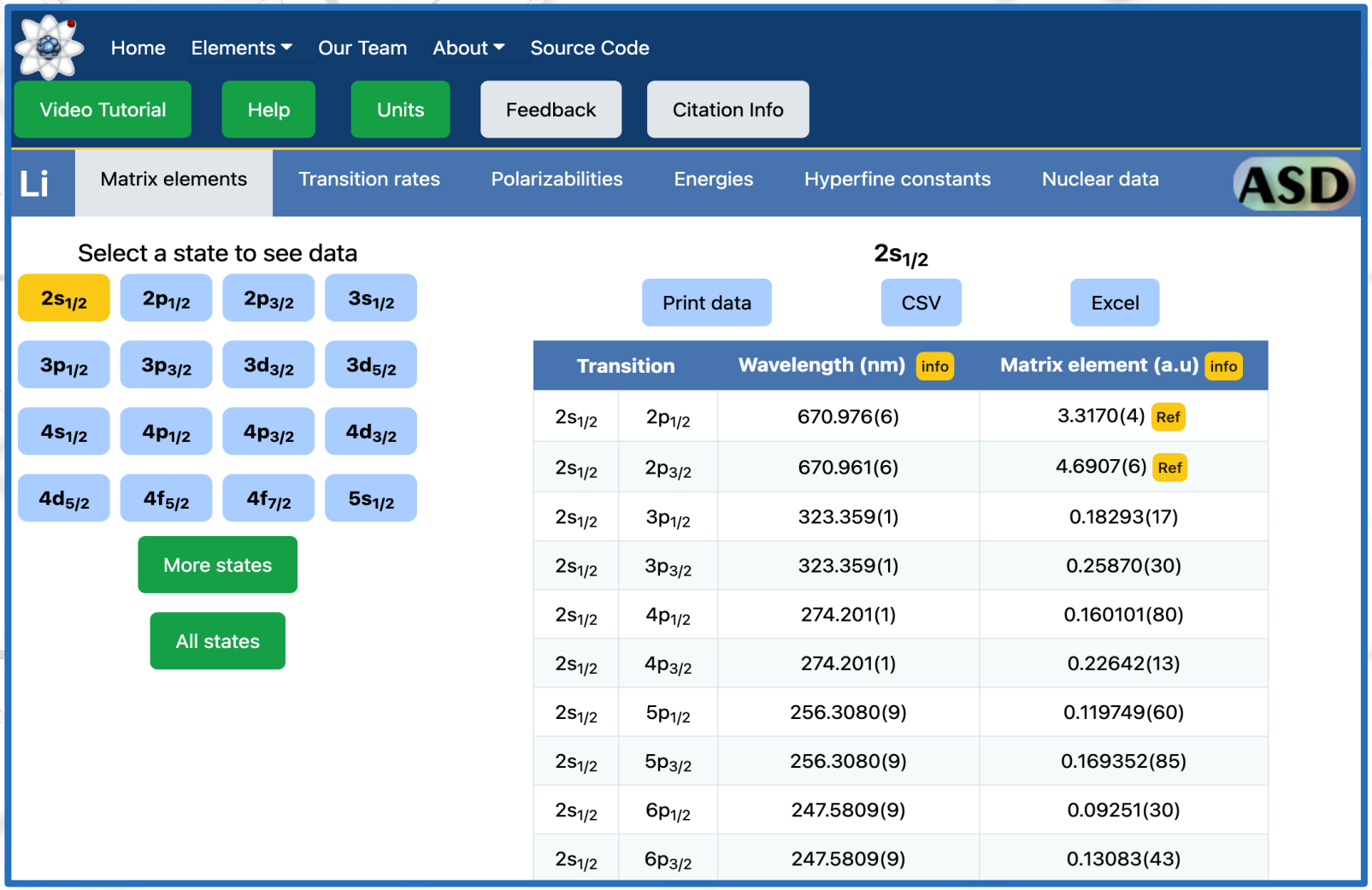
- One year into the project
- 2 Full-time RSEs newly hired
- Many proposed research projects, evaluated and
- Student RSEs engaged and working on projects as well
  - Several student volunteers from Master's in Data Science program
- Initial RSE course to be offered in Spring 2026
- Workshops in mid-Atlantic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

The Atom Project – CSSI award 2209639

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



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

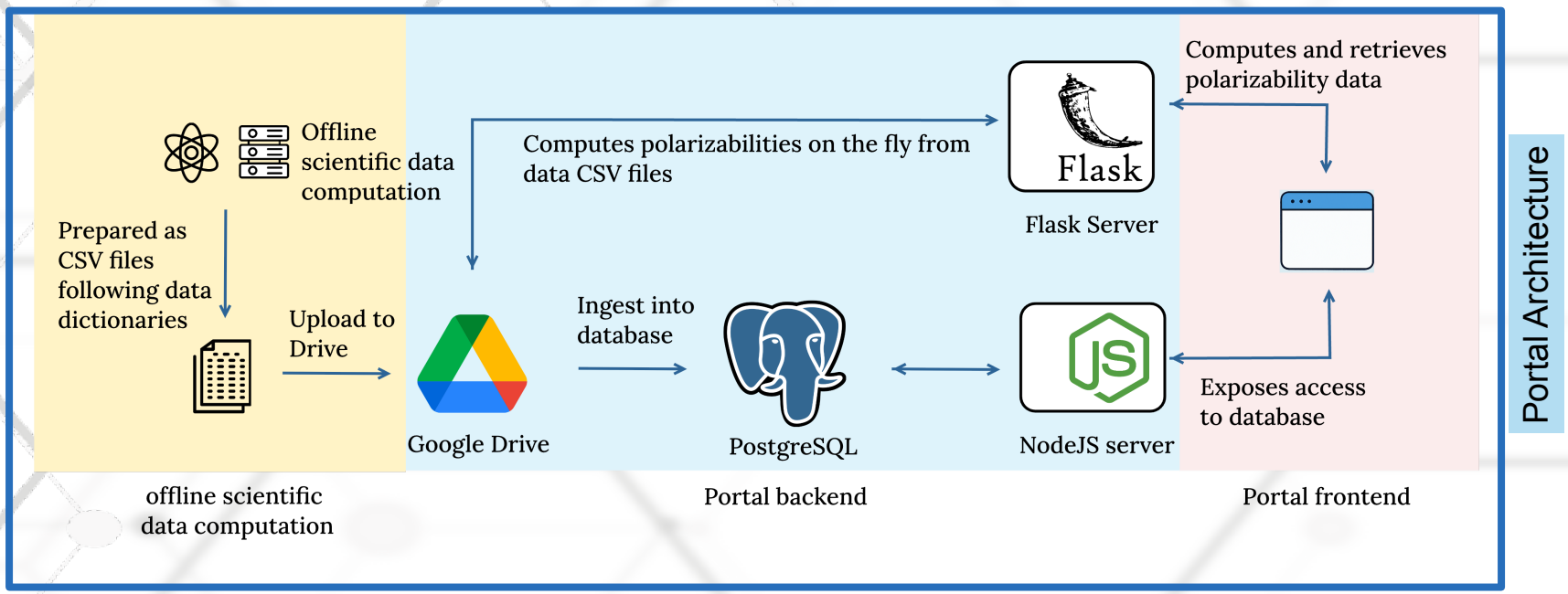


Transition		Wavelength (nm) info	Matrix element (a.u) info
$2s_{1/2}$	$2p_{1/2}$	670.976(6)	3.3170(4) Ref
$2s_{1/2}$	$2p_{3/2}$	670.961(6)	4.6907(6) Ref
$2s_{1/2}$	$3p_{1/2}$	323.359(1)	0.18293(17)
$2s_{1/2}$	$3p_{3/2}$	323.359(1)	0.25870(30)
$2s_{1/2}$	$4p_{1/2}$	274.201(1)	0.160101(80)
$2s_{1/2}$	$4p_{3/2}$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

Atom Portal – Data Example: Polarizability Graphs

Atom Portal: Challenges on the Computer Science Side

- Automating web page generation from physics data

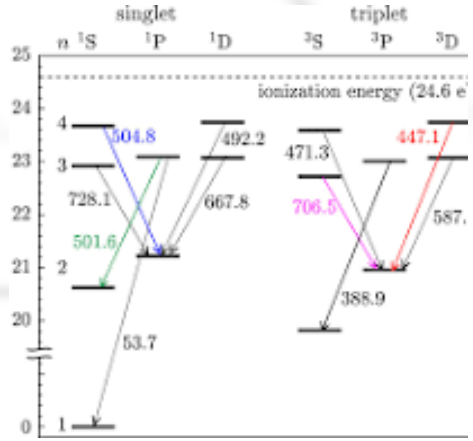


- Collaboration with physicists

Atom Portal Project: Status and What's Next?

Portal Version 3 released in June 2025:

- 28 atoms/ions
- Energies, transition matrix elements, transition rates, radiati
  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

- UD AI Center of Excellence
- XAI - out of distribution data - e.g. extreme weather events
- First State AI Institute

Thanks for Listening !

Any Questions

Contact us. darse-scipe@udel.edu