

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



Democratizing Access to Research Software
Engineering

SCIPe award 2417814

Rudi Eigenmann, University of Delaware



Who is Involved ?

UD Leadership

PI



Sunita Chandrasekaran
Associate Professor
Computer & Info Sciences
Vice Chair State of DE AI
commission



Rudi Eigenmann
Professor
Electrical & Computer
Engineering



Tian-Jian Hsu
Professor
Civil & Environmental
Engineering



Benjamin Bagozzi
Professor
Political Science &
Internat. Relations



John Huffman
Director
Research Computing

Howard



Rajni Goel
Professor, Information
Systems & Supply Chain
Management

DSU



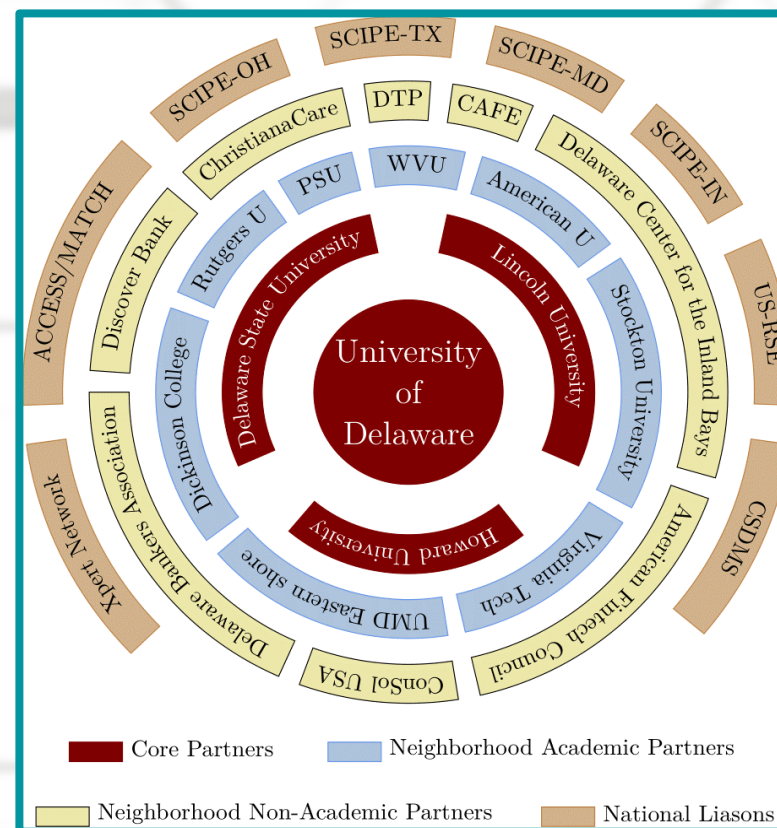
Gulnihal Ozbay
Associate Dean,
Cooperative
Extension &
Applied Research

Lincoln



Dejene Dedefa
Assistant Professor
Computer Science

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 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



Synchronizing 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

- 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



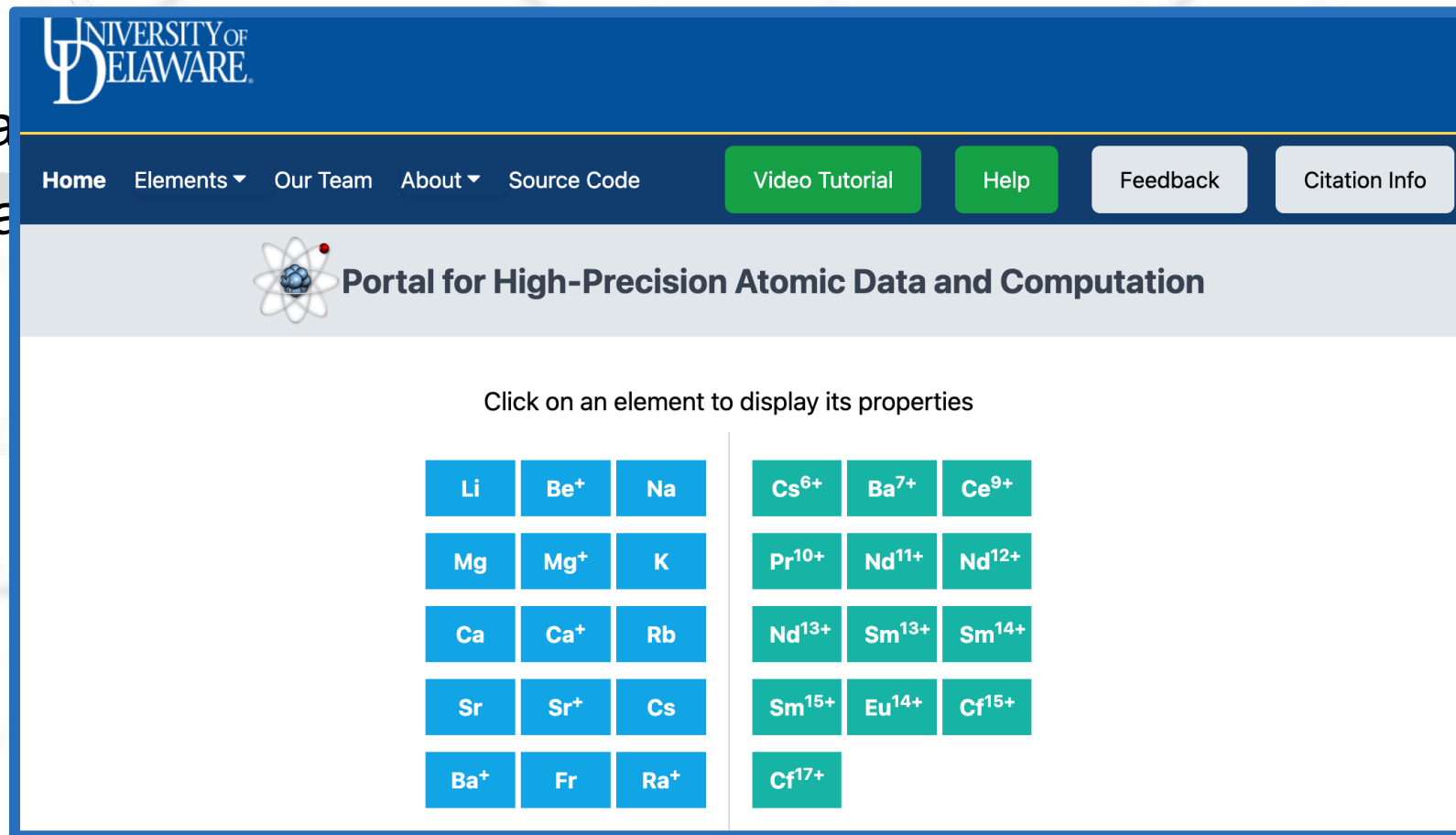
DARSE Project Status and What's Next ?

- 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



The screenshot shows the homepage of the 'Portal for High-Precision Atomic Data and Computation' at the University of Delaware. The header features the university's logo and a navigation bar with links: Home, Elements (dropdown), Our Team, About (dropdown), Source Code, Video Tutorial (highlighted in green), Help (highlighted in green), Feedback, and Citation Info. Below the navigation bar is a banner with an atomic symbol icon and the title 'Portal for High-Precision Atomic Data and Computation'. The main content area includes the instruction 'Click on an element to display its properties' and a periodic table of elements. The elements are displayed in two columns of colored boxes: blue for neutral atoms and green for ions. The first column (blue) includes Li, Be⁺, Na, Mg, Mg⁺, K, Ca, Ca⁺, Rb, Sr, Sr⁺, Cs, Ba⁺, Fr, and Ra⁺. The second column (green) includes Cs⁶⁺, Ba⁷⁺, Ce⁹⁺, Pr¹⁰⁺, Nd¹¹⁺, Nd¹²⁺, Nd¹³⁺, Sm¹³⁺, Sm¹⁴⁺, Sm¹⁵⁺, Eu¹⁴⁺, Cf¹⁵⁺, and Cf¹⁷⁺.



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

Atom Portal interface showing data for the $2s_{1/2}$ state of Lithium (Li).

Navigation: Home, Elements, Our Team, About, Source Code

Buttons: Video Tutorial, Help, Units, Feedback, Citation Info

Li | Matrix elements | Transition rates | Polarizabilities | Energies | Hyperfine constants | Nuclear data | ASD

Select a state to see data

Buttons for states: $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, $3s_{1/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, $3d_{5/2}$, $4s_{1/2}$, $4p_{1/2}$, $4p_{3/2}$, $4d_{3/2}$, $4d_{5/2}$, $4f_{5/2}$, $4f_{7/2}$, $5s_{1/2}$

Buttons: More states, All states

Print data, CSV, Excel

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)	

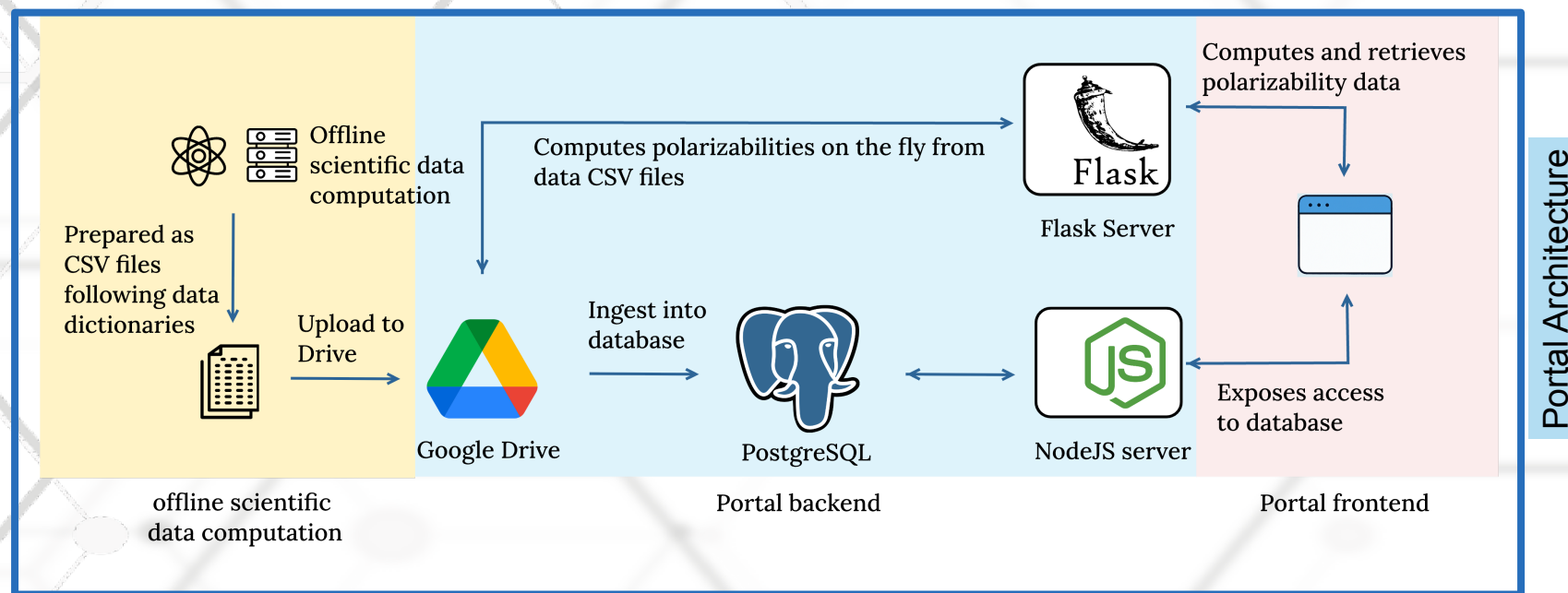


Atom Portal – Data Example: Polarizability Graphs



Atom Portal: Challenges on the Computer Science Side

- Automating web page generation from physics data



- Collaboration with physicists



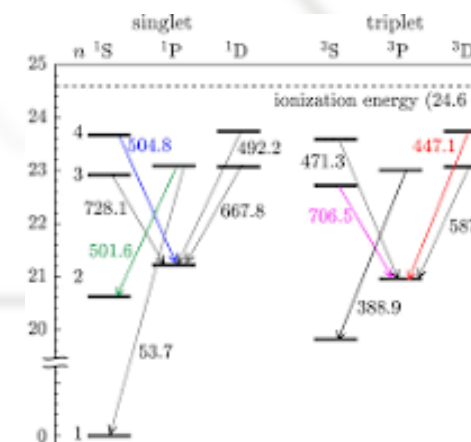
Atom Portal Project: Status and What's Next?

Portal Version 3 released in June 2025:

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

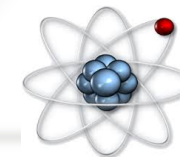
Next

- 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

