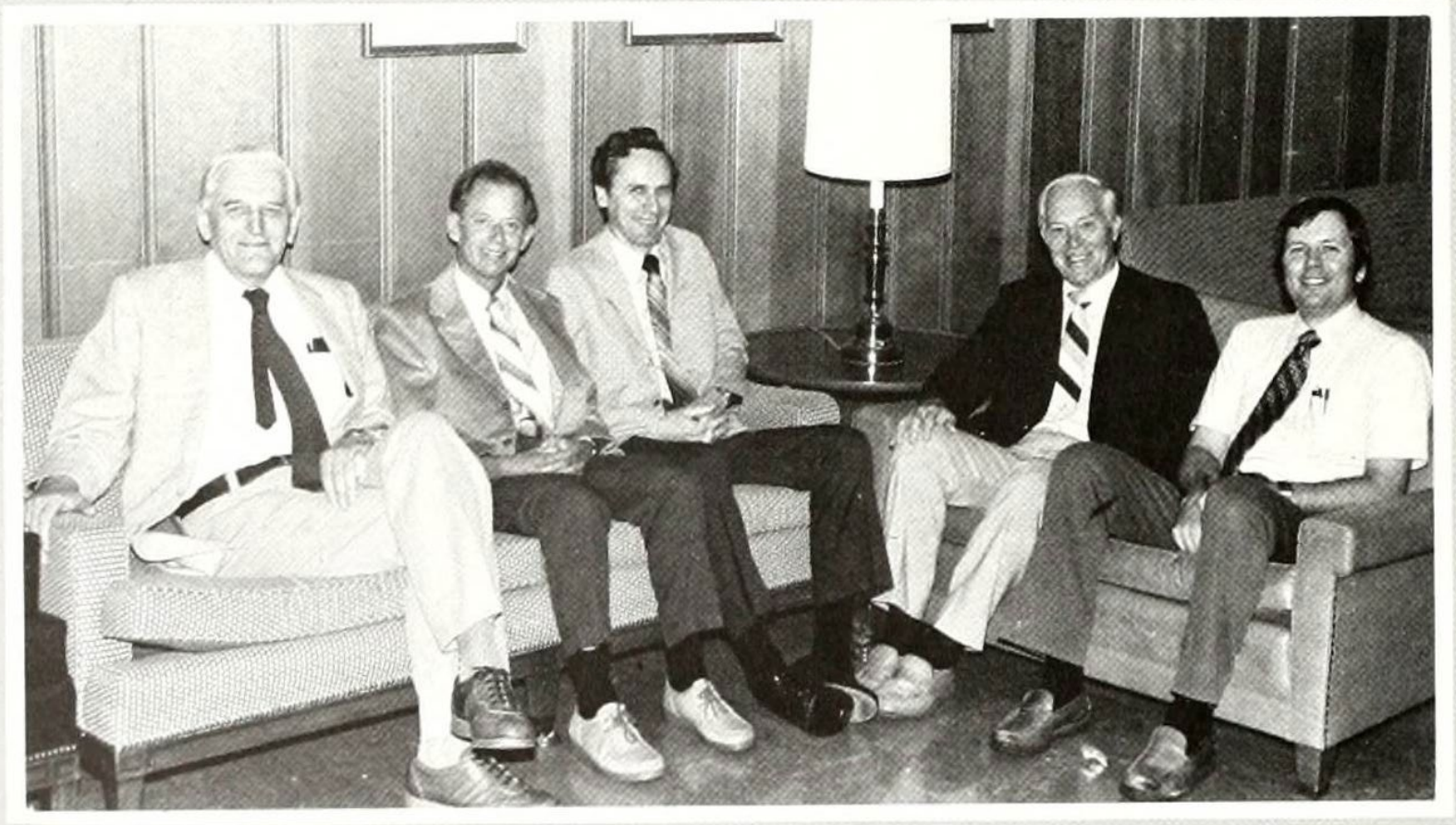
Perspective on WFU Physics Part 2
Natalie Holzwarth

- ❑ Some recollections about WFU Physics Department 1983++
- ❑ Recollections of great collaborations
- ❑ Some observations about the trajectory of physics generally and the field of computational materials science more specifically
- ❑ Some opinions

Some recollections about WFU Physics Department 1983++

Physics

From 1983 Howler Yearbook



Brooke Reinhardt

Ysbrand Haven, Robert Brehme, William Kerr, George Williams, George Matthews.

Howard Shields

More Howler Yearbook photos from Rick Matthews

Escaping Salem Hall to move into Olin Physical Laboratory in 1989

More Howler Yearbook photos from Rick Matthews

(Not sure how Rick managed to take us to Mars this year)

What makes the WFU physics department so successful?

- Hard work and focus (+ (perhaps) good luck)
- A climate of collaboration among students and faculty
- Weekly colloquium series
- Regular topical seminar series
- SPS, Physics T-shirts, other social activities
- Refreshments

Recollections of great collaborations

Undergraduate honors:

Christopher Kimmer 1995
Cameron Kates 2014
James Drewery 2014
Hannah Zhang 2015

Masters of science:

Jeffrey Gardner 1986
Qingsheng Wang 1989
Larry Rush, Jr. 2017

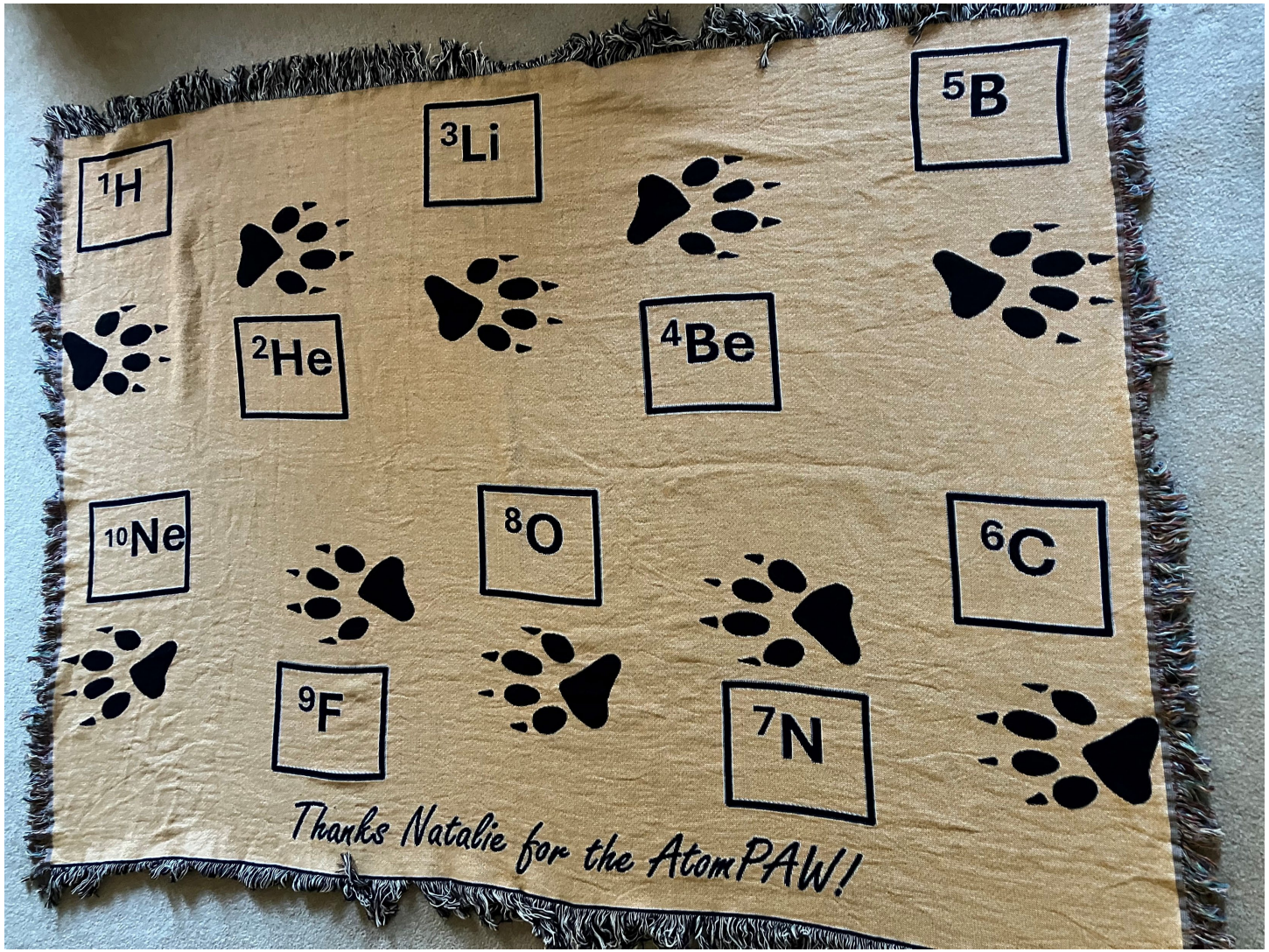
Faculty Co-authors:

Rick Matthew
Richard Williams
Bill Kerr
Abdou Lachgar, Cynthia Day, and Mike Gross

Doctors of Philosophy:

Yueping Zeng 1997
Alan Tackett 1998
(Rick Matthews collaborating mentor)
Yonas Abraham 2004
(Richard Williams collaborating mentor)
Ping Tang 2006
Kevin Conley 2008
Xiao Xu 2011
Nicholas Lepley 2015
Jason Howard 2018
Ahmad Al-Qawasmeh 2018
Yan Li 2021
Dominique Itanze 2024
(Scott Geyer collaborating mentor)
D. Cory Lynch 2025 (expected)

Appreciation and gratitude for surprise present received a few months ago – wonderful collaboration by several alums --



Wanyi Nie
Chaochao Dun
Hannah Zhang
Yaochuan Mei
Yan Li
Xiao Xu
Yuan Li
Leo Ding
Chen Liu
Qi Li
Jie Liu
Rongzhong Li
Xinfu Lu
Xiaohua Liu
Wenxiao Huang
Jiajie Xiao

Some thoughts on the trajectory of physics

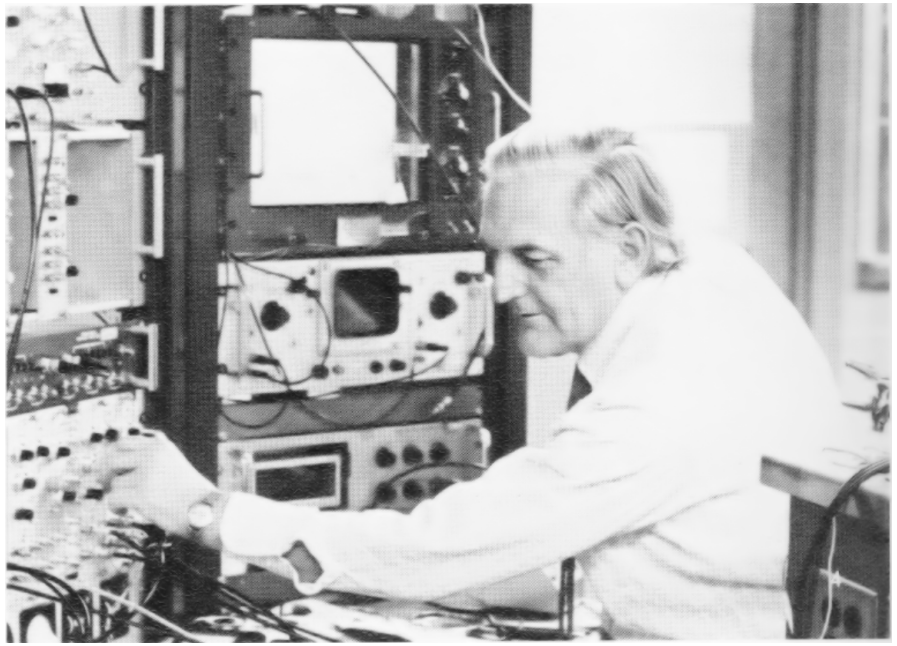
- Development of ideas is not always progressive –
  - Sometimes it is worth revisiting old ideas

An example special to WFU – ionic conductivity

- Studied by Ysbrand Haven ~1950-1983
- With the technological push to find better battery materials, Haven's work is again popular

Ysbrand Haven –
WFU Physics Professor 1965-1983

1975 Howler photo of Professor Haven with his conductivity equipment.



Studied ionic conductivity in well-controlled crystalline samples as a function of temperature, to develop models of basic mechanisms and their relationship to diffusion.

Ionic conductivity in LiI (single crystal form)

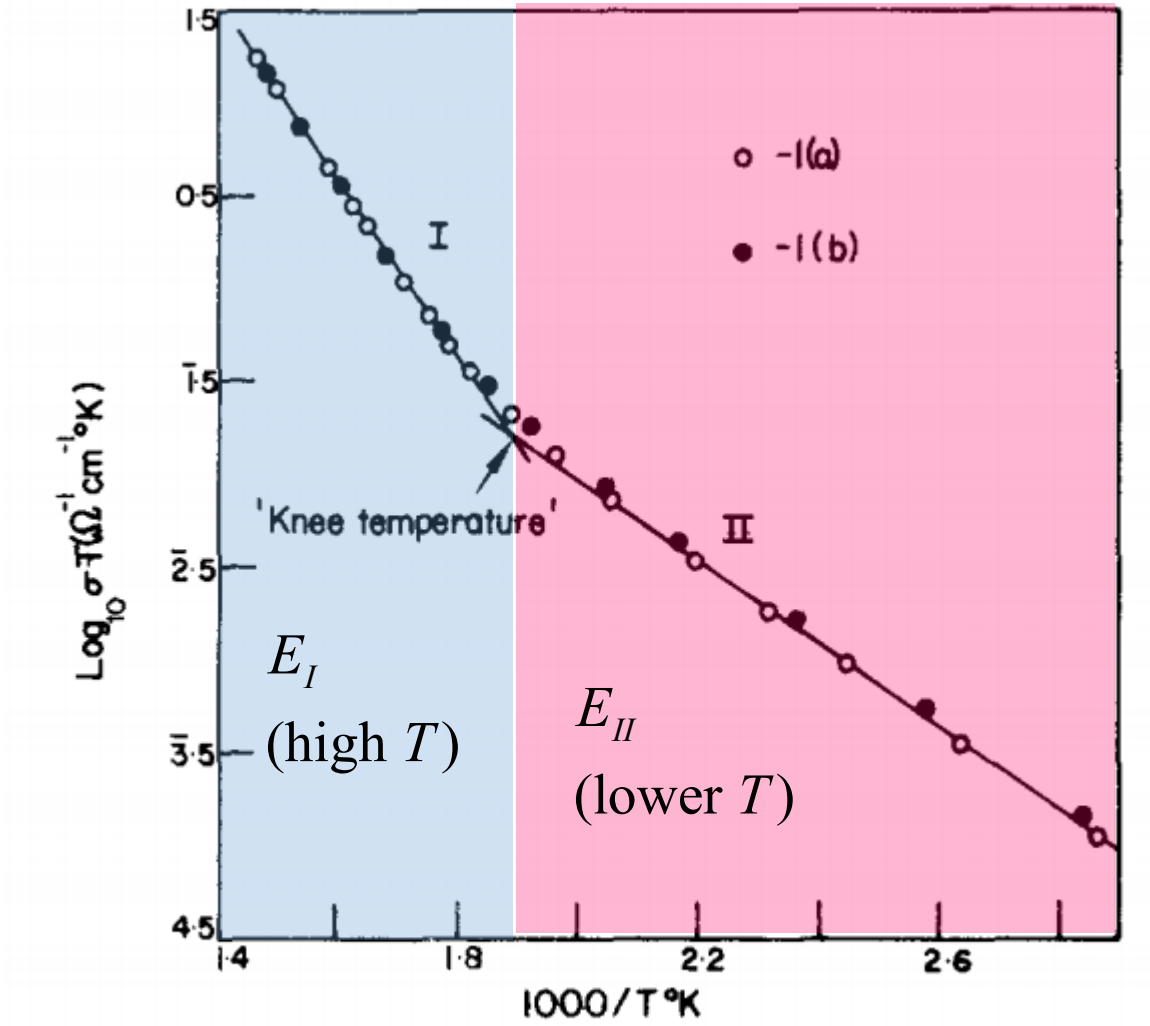


Fig. 2. The intrinsic (I) and extrinsic (II) regions of the ionic conductivity plot for two specimens of as-grown material.

B. J. H. Jackson and D. A. Young, J. Phys. Chem. Solids 30, 1973-1976 (1969)

$$\sigma = \frac{K_I}{T} e^{-E_I/k_B T} + \frac{K_{II}}{T} e^{-E_{II}/k_B T}$$

E_I and E_{II} are "activation" energies, characteristic of the hopping processes.

Relationship between ionic conductivity and diffusion

From statistical mechanics

(Nernst-Einstein relation)

$$\sigma = \frac{N}{V}\frac{q^2}{k_B T} D^{(\text{all})}$$

$$= \frac{1}{H_r}\frac{N}{V}\frac{q^2}{k_B T} D^{(\text{tracer})}$$

Haven ratio: $H_r = \dfrac{D^{(\text{tracer})}}{D^{(\text{all})}}$

Key:

$\sigma \equiv$ DC electrical conductivity

$D \equiv$ Diffusion coefficient

$\frac{N}{V} \equiv$ #mobile ions per unit volume

$q \equiv$ charge of mobile ions

$k_B \equiv$ Boltzmann constant

$T \equiv$ temperature in Kelvin

$D^{(\text{tracer})}$: can be measured using nuclear isotopes; represents independent particle motions
accessible by computation

$D^{(\text{all})}$: measured from the conductivity; includes correlated motions of mobile ions
very difficult to compute

Some reflections on the trajectory of computational materials physics Historically

Equations

$$E_x^{avv} - \tilde{E}_x^{avv} = -\sum_{vv'} \sum_{L=|l_v-l'_v|}^{l_v+l'_v} \frac{1}{2}\Theta_{vv'}^{L} \sum_{ijkl} \langle \tilde{\Psi}_v^{\mathrm{HF}} | \tilde{P}_i^a \rangle \langle \tilde{P}_j^a | \tilde{\Psi}_{v'}^{\mathrm{HF}} \rangle$$

$$\times \langle \tilde{\Psi}_{v'}^{\mathrm{HF}} | \tilde{P}_k^a \rangle \langle \tilde{P}_l^a | \tilde{\Psi}_v^{\mathrm{HF}} \rangle (R_{ij;kl}^{aL} - \tilde{R}_{ij;kl}^{aL}) \qquad (61)$$

and

$$E_x^{acv} - \tilde{E}_x^{acv} = -\sum_{vc} \sum_{L=|l_v-l_c|}^{l_v+l_c} \Theta_{vc}^{L} \sum_{ij} \langle \tilde{\Psi}_v^{\mathrm{HF}} | \tilde{P}_i^a \rangle \langle \tilde{P}_j^a | \tilde{\Psi}_v^{\mathrm{HF}} \rangle$$

$$\times (R_{ic;cj}^{aL} - \tilde{R}_{ic;cj}^{aL}). \qquad (62)$$

Here

$$R_{ij;kl}^{aL} \equiv e^2 \int\int dr\, dr' \frac{r_<^L}{r_>^{L+1}} \phi_i^{a*}(r) \phi_j^a(r) \phi_k^{a*}(r') \phi_l^a(r') \qquad (63)$$

and

$$\tilde{R}_{ij;kl}^{aL} \equiv e^2 \int\int dr\; dr' \frac{r_<^L}{r_>^{L+1}} [\tilde{\phi}_i^{a*}(r) \tilde{\phi}_j^a(r) + \hat{m}_{ij}^{aL}(r)]$$

$$\times [\tilde{\phi}_k^{a*}(r') \tilde{\phi}_l^a(r') + \hat{m}_{kl}^{aL}(r')]. \qquad (64)$$

Code

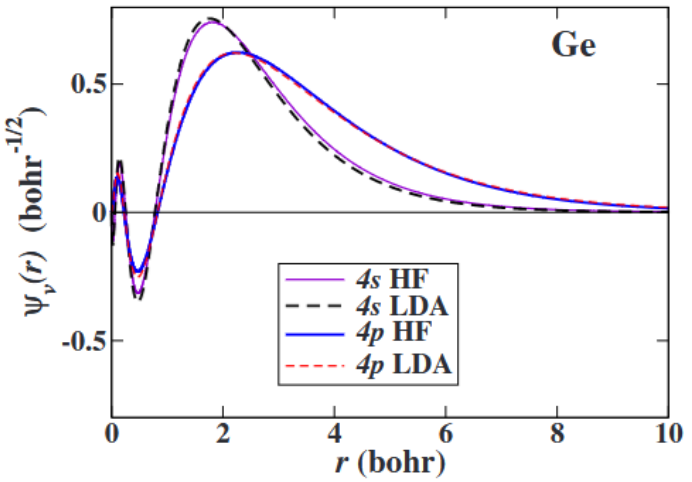
```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!  Program uses two grids -- "universal grid" Grid
!   and modified grid Grids, with fixed Grids%n=401 and ns=400
!     and Grids%r0=0.1 which are found to work well for splinesolver
!   Internally need to omit origin and so ns=Grids%n-1
!   For MGGA case (needvtau=.true.) also need fine linear grid
!      Gridf
!  Setup local private grid
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
  SUBROUTINE initsplinesolver(Grid,splns,splr0)
    Type(GridInfo), INTENT(IN) :: Grid      !Input universal grid
    INTEGER, INTENT(IN) :: splns  !spline grid
    REAL(8), INTENT(IN) :: splr0  !spline r0
    INTEGER :: i,nf
    REAL(8) :: hf,x

    !r0=0.1d0    ! 0.1 seems to be a good idea
    !ns=400      ! seems to be good enough
    r0=splr0
    ns=splns
    h=log(1.d0+Grid%r(Grid%n)/r0)/ns
    call initgridwithn(Grids,2,ns+1,r0,h)  !local loggrid

    write(std_out,*) 'initsplinesolve ', r0,ns,h;call flush_unit(std_out)

    allocate(u(ns+1),pref(ns+1),rr1(ns+1),rr2(ns+1))
    allocate(srv(ns+1),svtau(ns+1),sdvt(ns+1))
    allocate(soneplusvt(ns+1))
    do i=1,ns+1
:
```

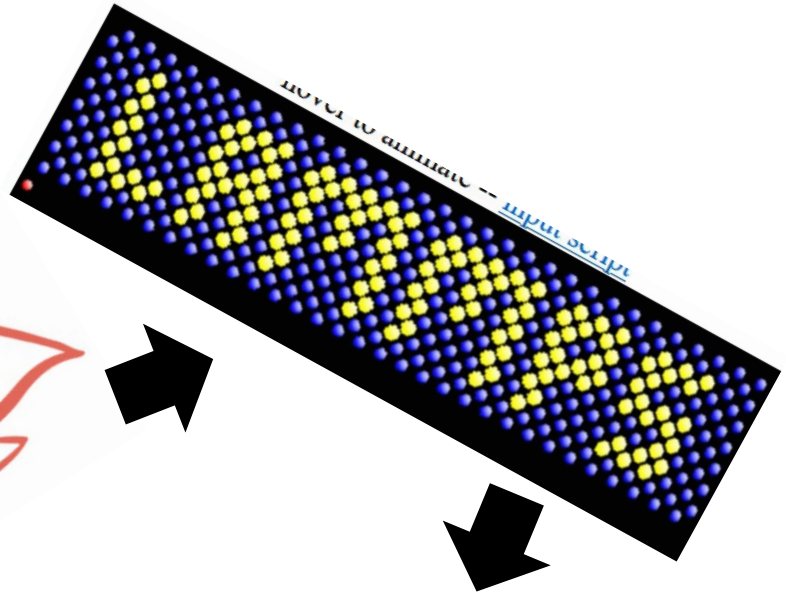
Results

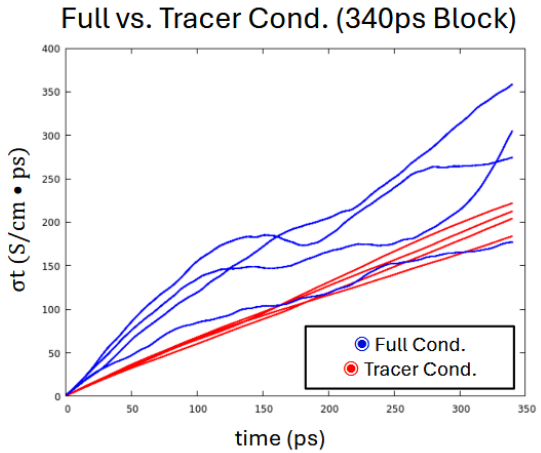


Some reflections on the trajectory of computational materials physics

Typical materials focused project in 2025

Input data





Results

Some reflections on the trajectory of computational materials physics

Code developers

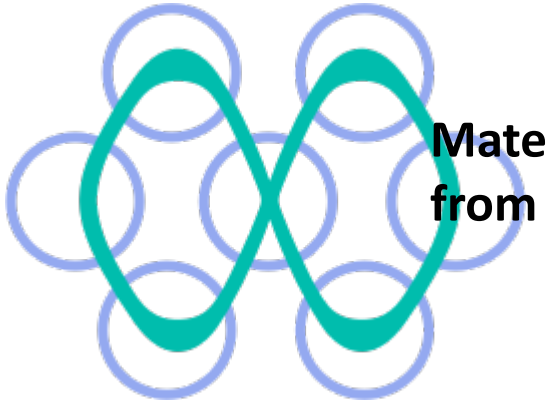
QUANTUMESPRESSO

Abinit

FHI-aims
The ab initio materials simulation package

b-initio VASP ienna imulation ackage

Materials studies



Materials Project from Berkeley Labs

Northwestern U

High throughput investigations; often barely mentioning software used for study

Some reflections on the trajectory of computational materials physics

Natalie's concerns about using code packages

1. Will code users lose their programing and algorithmic development skills?
2. Will code users forget to scrutinize the results? Every once in a while it might be good check results with two different codes.
3. Will code developers have time to also do materials focused projects?

Advice: If you do use a code package, become an active user, participating in the package community discussions, asking questions, providing feedback, etc.

Some opinions –

We find ourselves in a frightening time in which normal academic activities, including science, is under attack by some. Natalie hopes to “keep calm and carry on”, striving to always maintain the intellectual and moral high ground. We are very lucky that Maxwell’s equations and Newton’s laws are not likely to fall into disfavor because they are contrary to someone’s vision of America. We just need to figure out how to restore rational thought processes more generally throughout the country.