Workshop on Computational *Ab initio* Quantum Thermodynamics

Qi Zhang[1], *Renata Wentzcovitch*[1,2,3]

Nov. 28 – Dec. 1, 2022

1. Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY
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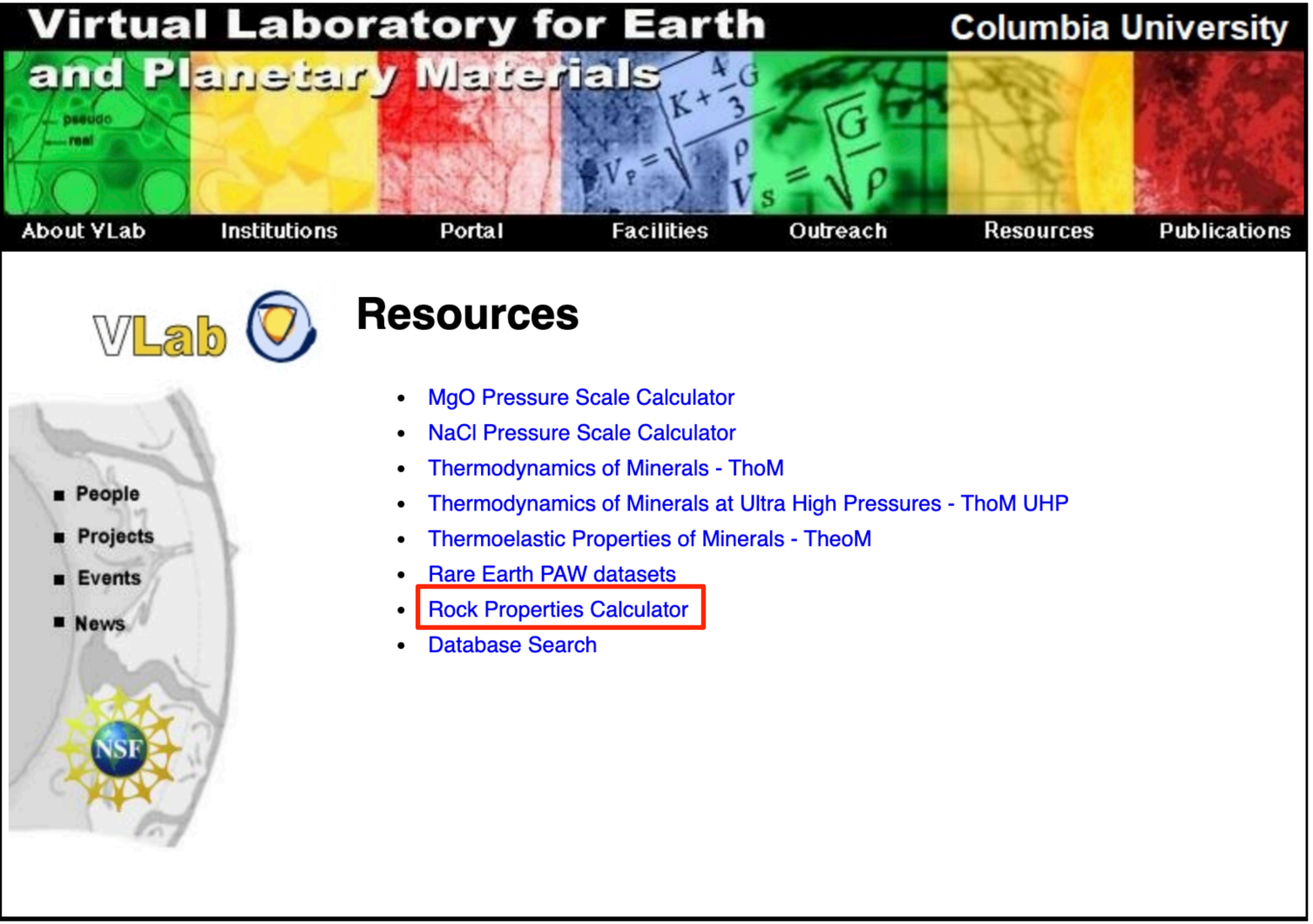
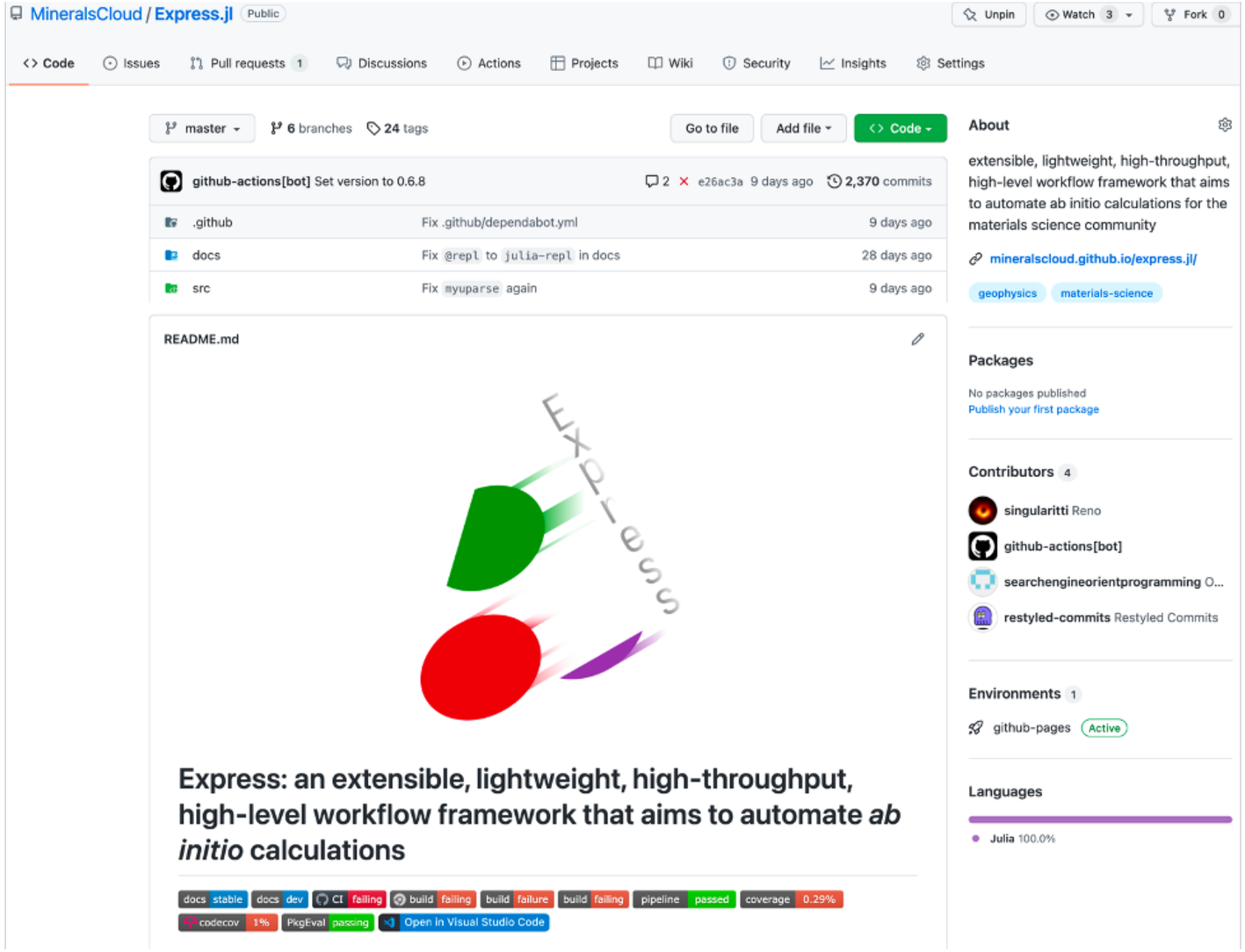


Predecessor

- The **V**irtual **Lab**oratory for Earth and Planetary Materials (VLab), was funded by the NSF in 2004 at the Minnesota Supercomputing Institute, University of Minnesota.
- VLab is a cyberinfrastructure consisting a fully integrated web portal, web services, and databases for *ab initio* calculations of planetary materials.

C. R. S. da Silva et al. Virtual laboratory for planetary materials: System service architecture overview. Phys Earth Planet In. 163, 321–332 (2007).

Access our code



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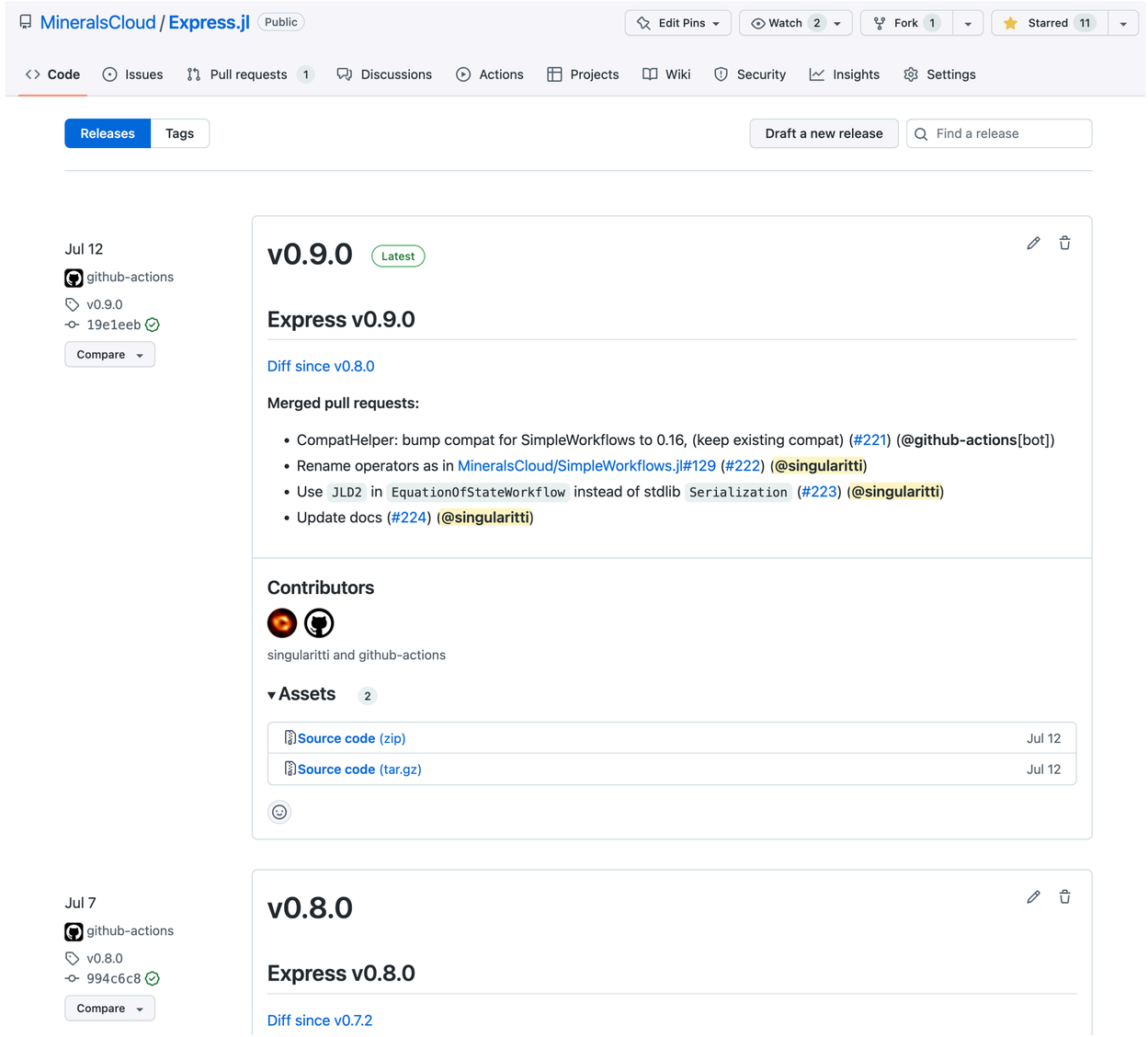

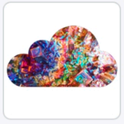

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We are a research team at Columbia University in the City of New York. Our Principal Investigator is Renata M. Wentzcovitch. Our research is devoted to computational quantum mechanical studies of materials at extreme conditions, especially planetary materials. We address electronic, structural, and vibrational properties from a fundamental and inter-related perspective.

Our current research interests include:

- Mineral physics with applications to geophysics (seismology and geodynamics) and geochemistry (water speciation and isotope fractionation in minerals)
- Materials discovery at (exo)planetary interior conditions
- H2O-ice physics
- Properties of strongly correlated oxides and their crystalline defects
- Spin crossover systems
- Simulations methods development

Latest Events

- Workshop on Computational Ab initio Quantum Thermodynamics (Nov. 28 -- Dec. 1, 2022)
- Bringing Research Excellence To Africa: Omololu Akin-Ojo
- Materials Simulations in Earth and Planetary Sciences Seminars
- International Workshop on Recent Developments in Electronic Structure Methods (ES22)
- 2022 US-Africa Initiative in Electronic Structure Workshop

Latest Code Releases

- Express.jl v0.9.0 (Source Code, released 4 months ago)	- QuantumESPRESSOExpress.jl v0.5.7 (Source Code, released 4 months ago)
- QuantumESPRESSOBase.jl v0.7.7 (Source Code, released 3 months ago)	- EquationsOfStateOfSolids.jl v0.4.2 (Source Code, released 7 months ago)
- qha Remove `seaborn` from deps (Source Code, released 3 weeks ago)	- cij 1.0.0-b4 (Source Code, released 7 months ago)
- phq 1.0.0 released! (Source Code, released 3 years ago)	- SimpleWorkflows.jl v0.22.0 (Source Code, released 1 day ago)
- CrystallographyBase.jl v0.7.0 (Source Code, released 3 months ago)	- EasyJobs.jl v0.3.0 (Source Code, released 2 days ago)

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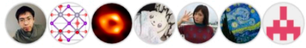

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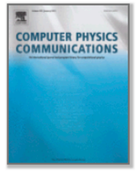

express: Extensible, high-level workflows for swifter *ab initio* materials modeling ☆, ☆☆

Qi Zhang [a], Chaoxuan Gu [a], Jingyi Zhuang [b, c], Renata M. Wentzcovitch [a, b, c]

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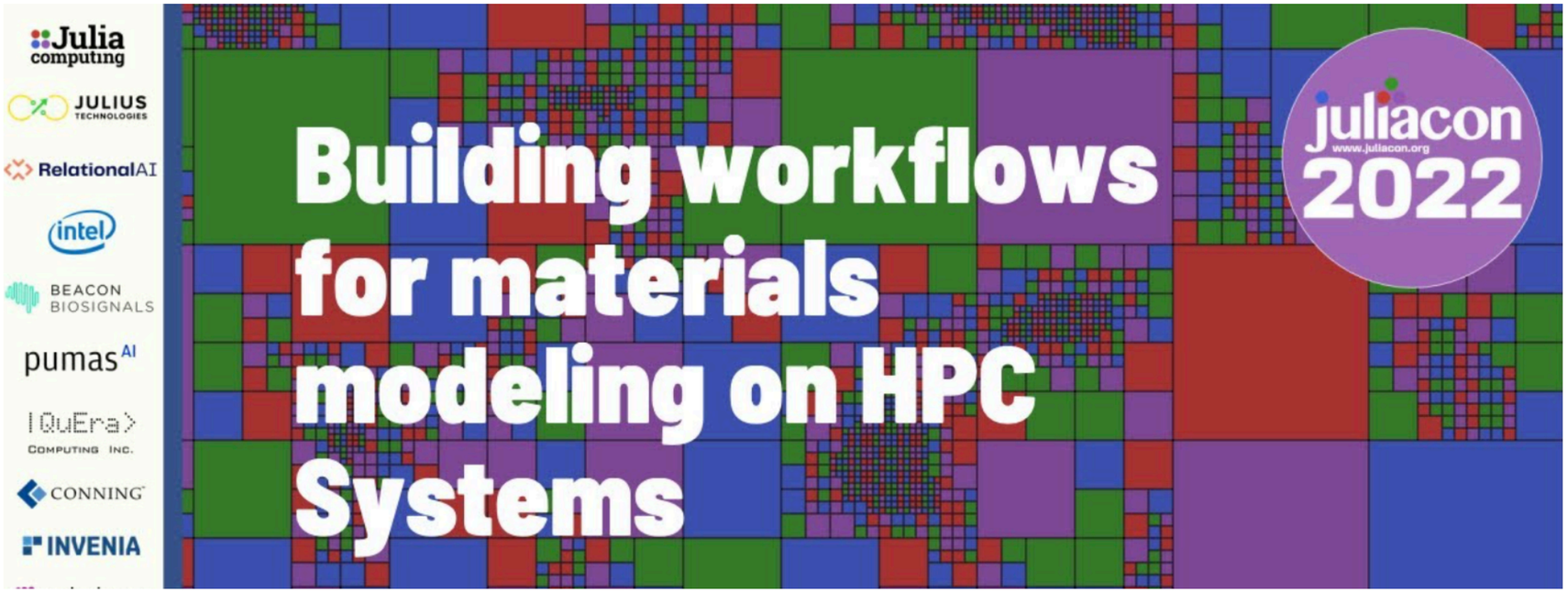
[Submitted on 24 Sep 2021]

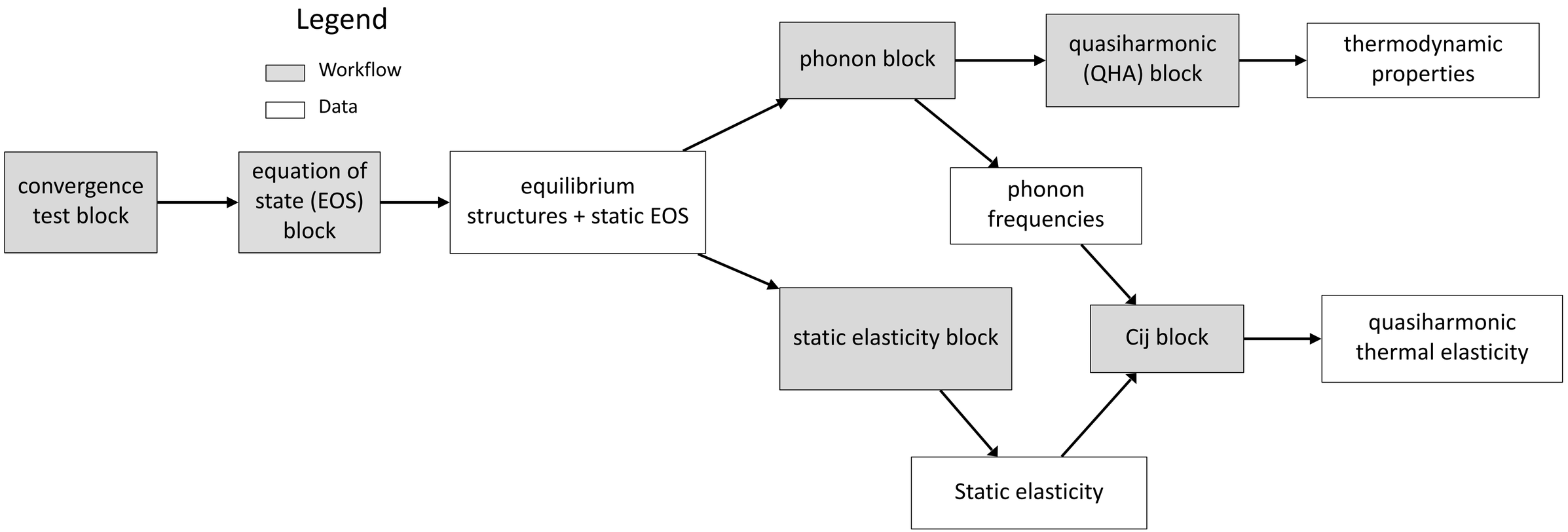
express: extensible, high-level workflows for swifter *ab initio* materials modeling

Qi Zhang (1), Chaoxuan Gu (1), Jingyi Zhuang (2 and 3), Renata M. Wentzcovitch (1 and 2 and 3) ((1) Department of

Details of the implementation

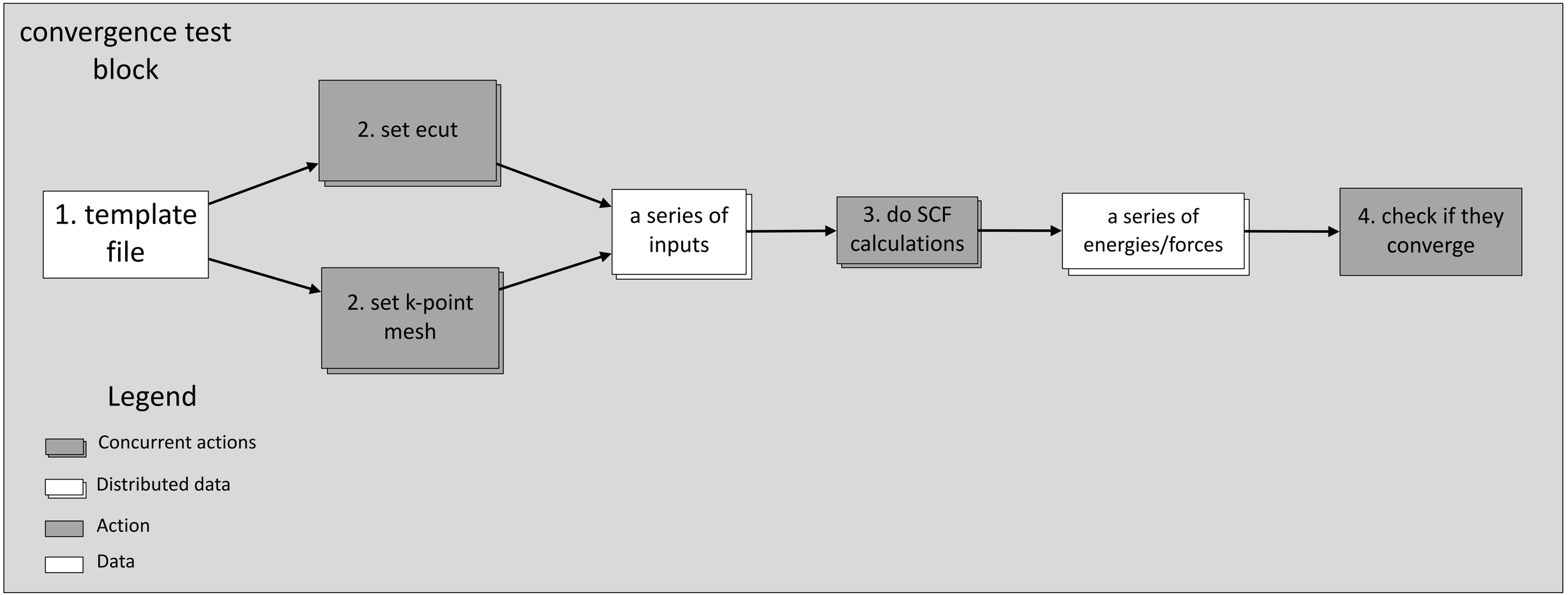


A high-level overview of the workflows



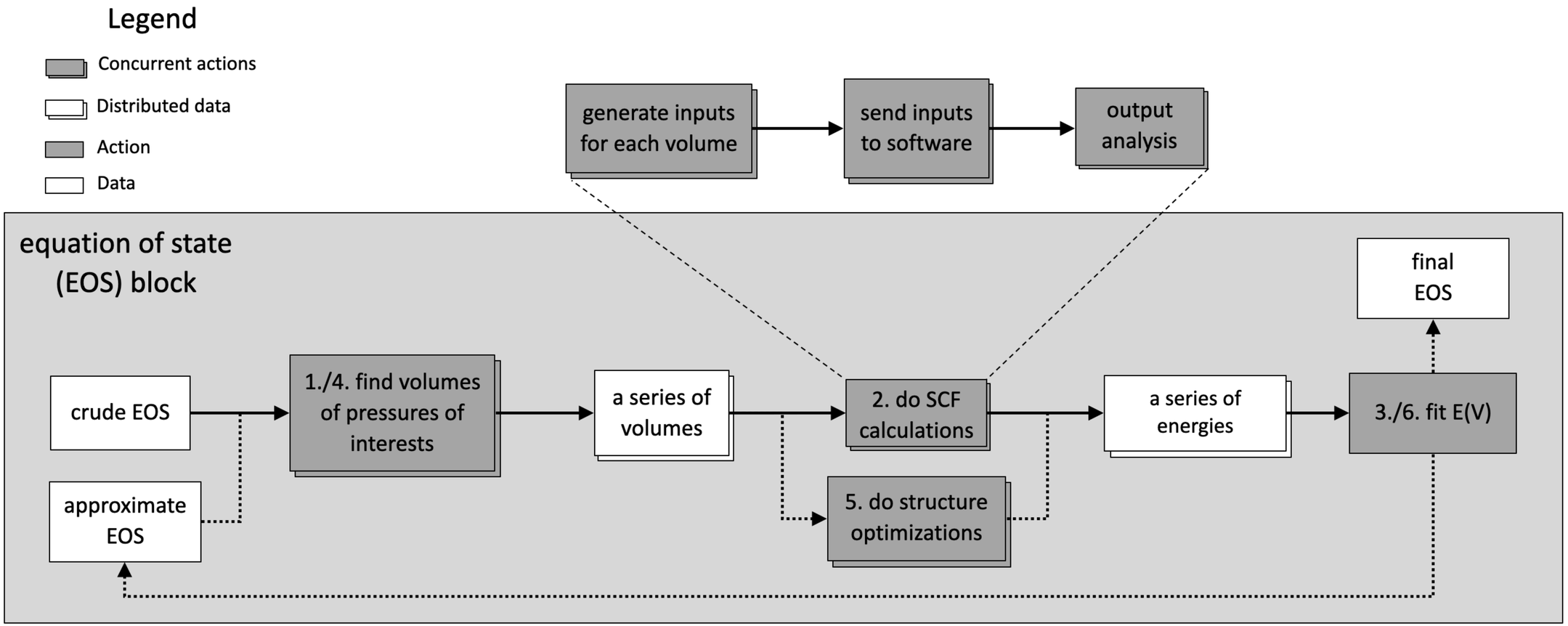
High-level schematic representation of the workflows. Each light-gray block denotes a workflow. A white block means the results obtained from a previous block. The cij block, colored as half-gray half-blue, is not currently contained in express but will be released in the near future.

Convergence test workflow



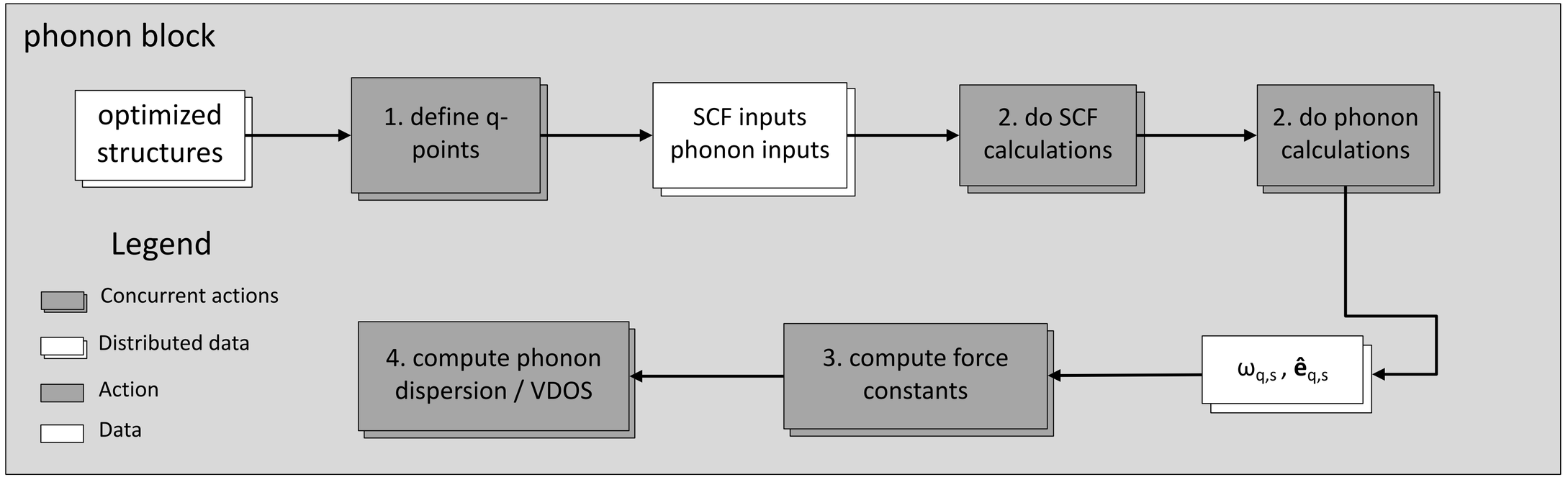
Schematic representation of the convergence test workflow.

Equation of state workflow



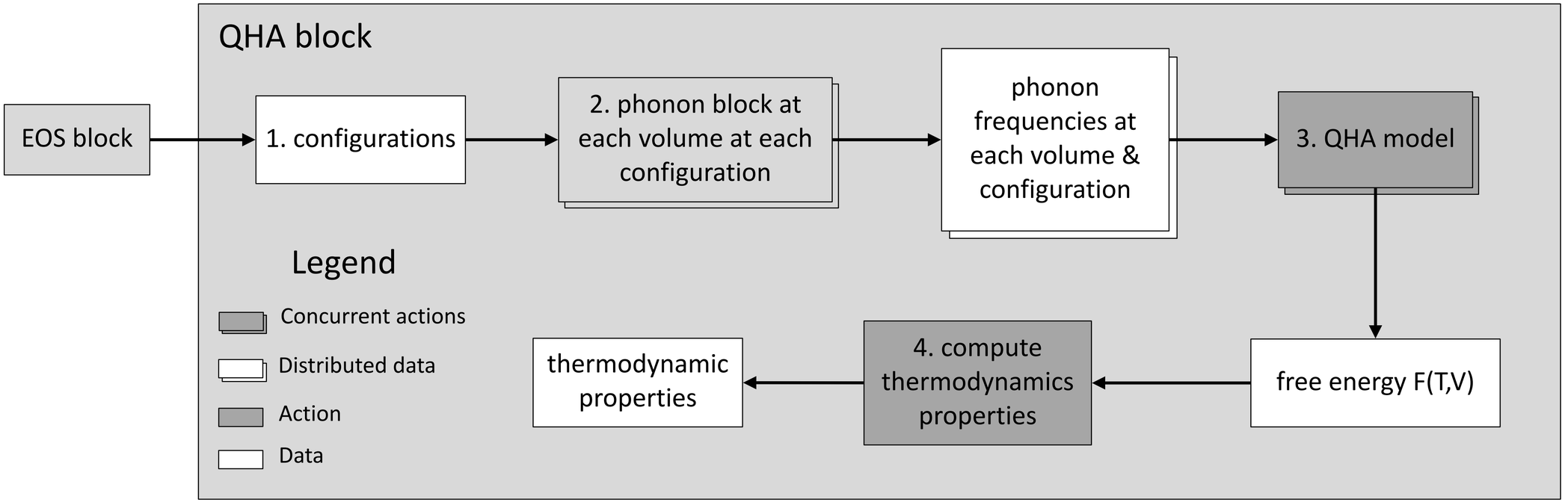
Visual depiction of the "parallel" implementation of the equation of state (EOS) workflow.

Phonon workflow



Graphical representation of the phonon workflow.

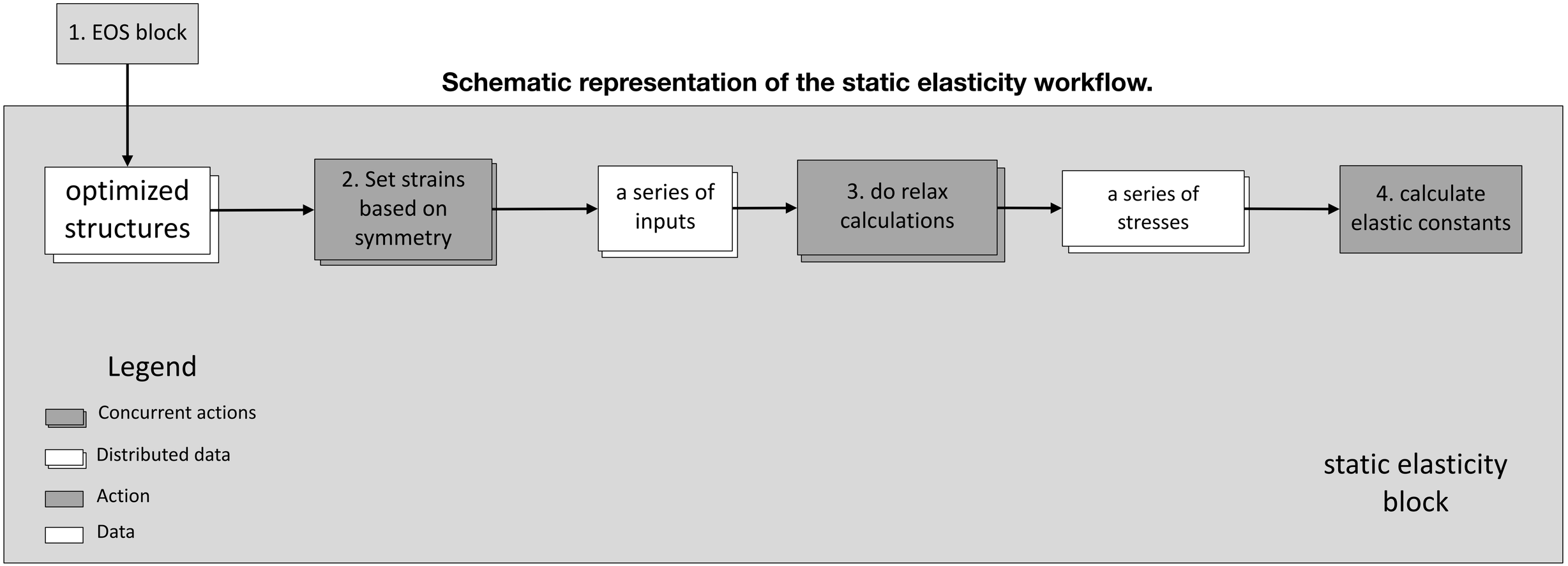
QHA workflow



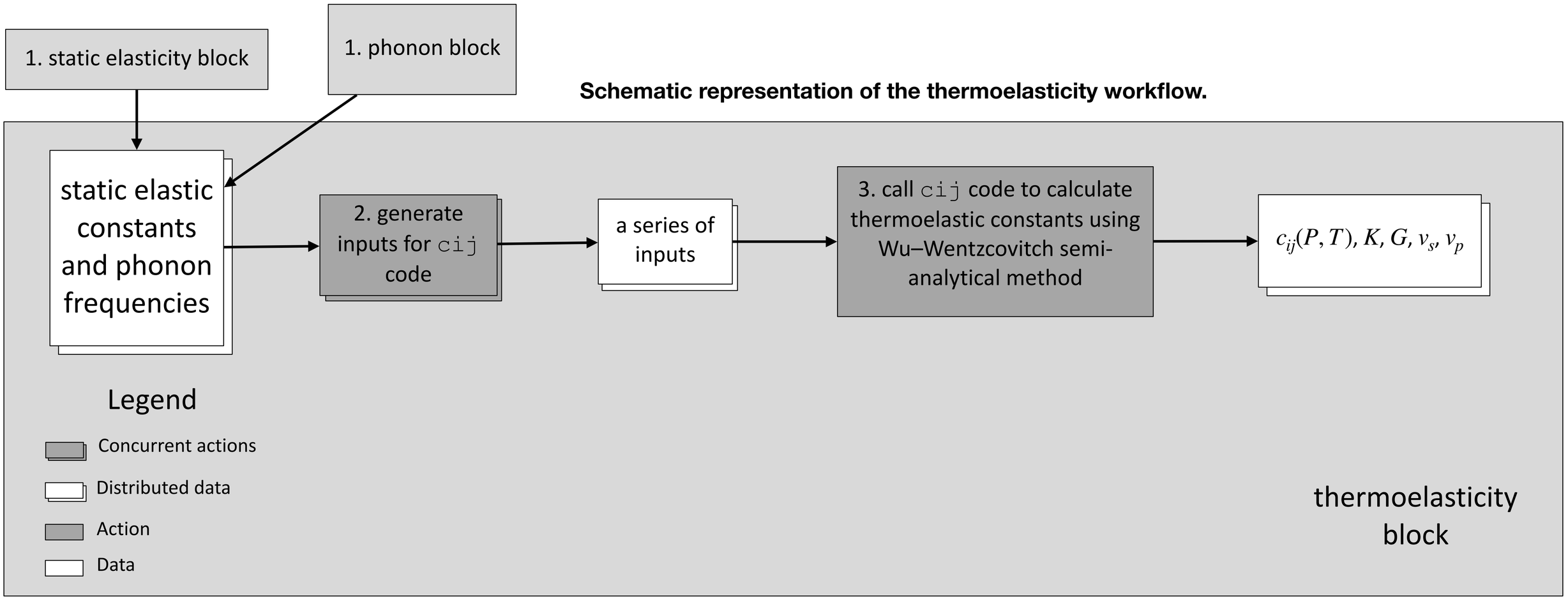
Schematic representation of the QHA workflow.

Qin, T., Zhang, Q., Wentzcovitch, R. M. & Umemoto, K. qha: A Python package for quasiharmonic free energy calculation for multi-configuration systems. *Comput Phys Commun* **237,** 199–207 (2019).

Static elasticity block



Thermoelasticity workflow



C. Luo, X. Deng, W. Wang, G. Shukla, Z. Wu, R. M. Wentzcovitch, cij: A Python code for quasiharmonic thermoelasticity. *Computer Physics Communications*. **267**, 108067 (2021).

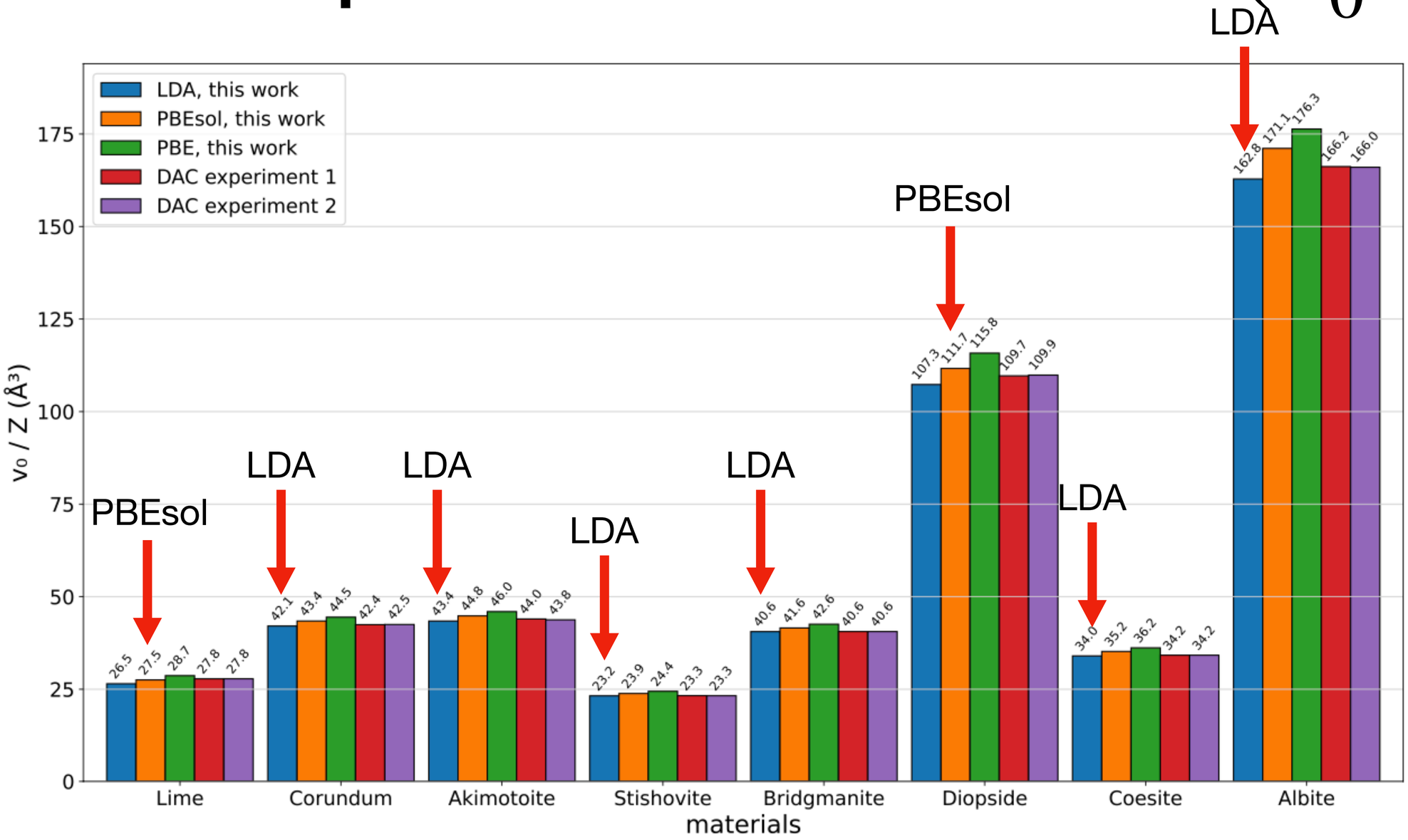
Crystal systems

Material	Formula	Space Group
Albite	$NaAlSi_3O_8$	$P\bar{1}$
Coesite	SiO_2	$C\frac{2}{c}$
Diopside	$CaMgSi_2O_6$	$C\frac{2}{c}$
Bridgmanite	$MgSiO_3$	Pbnm
Stishovite	SiO_2	$P\frac{4_2}{m}nm$
Akimotoite	$MgSiO_3$	$R\bar{3}$
Lime	CaO	$Fm\bar{3}m$
Corundum	Al_2O_3	$R\bar{3}c$

	LDA	PBEsol	PBE
O	O.pz-n-kjpaw_psl.0.1.UPF	O.pbesol-n-kjpaw_psl.1.0.0.UPF	O.pbe-n-kjpaw_psl.1.0.0.UPF
Al	Al.pz-n-kjpaw_psl.0.1.UPF	Al.pbesol-n-kjpaw_psl.1.0.0.UPF	Al.pbe-n-kjpaw_psl.1.0.0.UPF
Ca	Ca-pz.vdb	Ca.pbesol-spn-kjpaw_psl.1.0.0.UPF	Ca.pbe-spn-kjpaw_psl.1.0.0.UPF
Mg	Mg.pz-spnl-kjpaw_psl.1.0.0.UPF	Mg.pbesol-spnl-kjpaw_psl.1.0.0.UPF	Mg.pbe-spnl-kjpaw_psl.1.0.0.UPF
Na	Na.pz-spn-kjpaw_psl.0.2.UPF	Na.pbesol-spn-kjpaw_psl.1.0.0.UPF	Na.pbe-spn-kjpaw_psl.1.0.0.UPF
Si	Si.pz-n-kjpaw_psl.0.1.UPF	Si.pbesol-n-kjpaw_psl.1.0.0.UPF	Si.pbe-n-kjpaw_psl.1.0.0.UPF

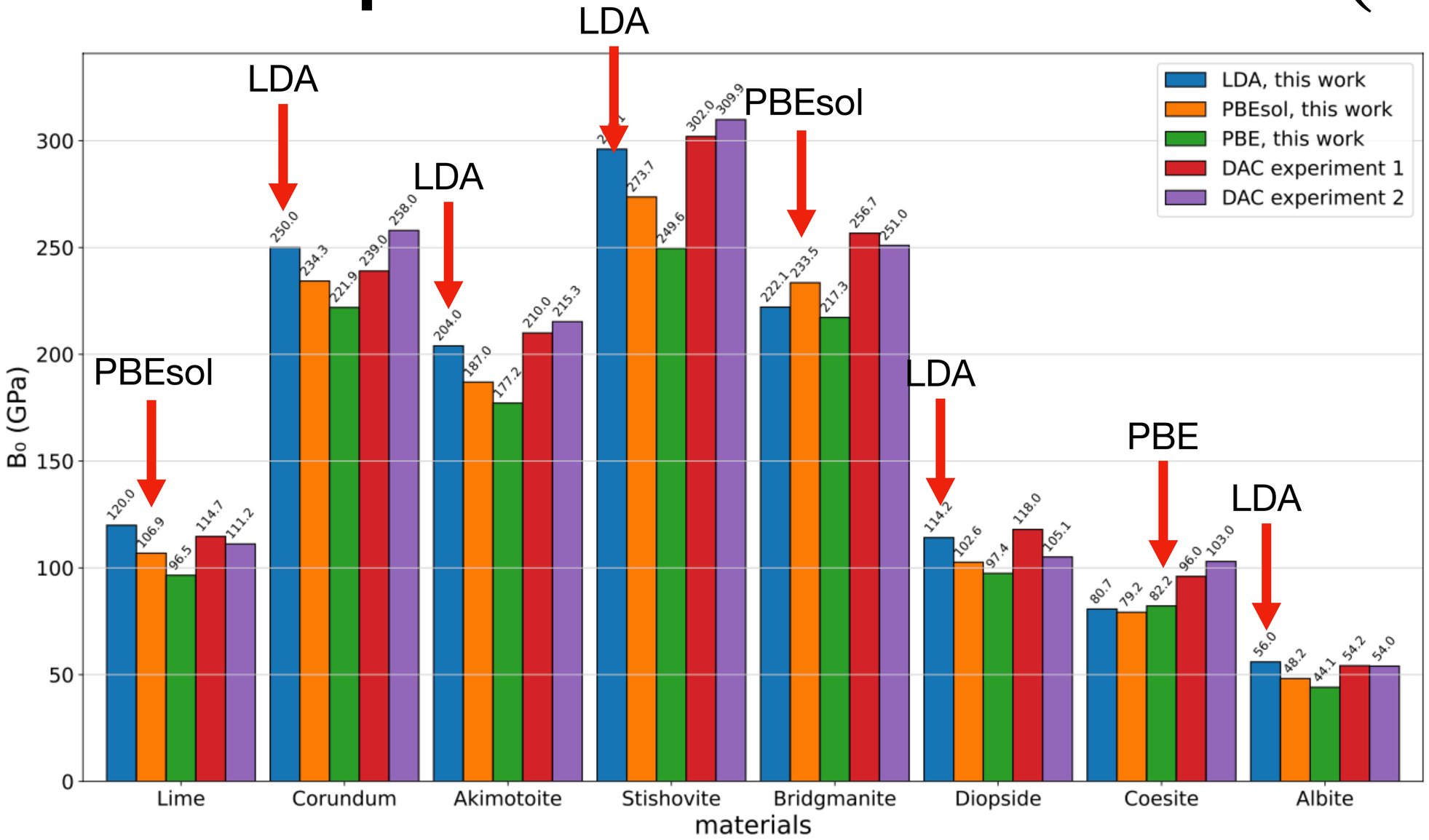
Material	Cutoff energy (Ry)			k-point mesh	q-mesh (DFPT)	q-mesh (sampling)
	LDA	PBEsol	PBE			
Albite	200	90	130	$2 \times 2 \times 2$	$2 \times 2 \times 2$	$20 \times 20 \times 20$
Coesite	110	90	130	$4 \times 4 \times 4$	$2 \times 2 \times 2$	$20 \times 20 \times 20$
Diopside	180	90	130	$4 \times 4 \times 4$	$2 \times 2 \times 2$	$20 \times 20 \times 20$
Bridgmanite	150	150	130	$6 \times 6 \times 4$	$2 \times 2 \times 2$	$20 \times 20 \times 20$
Stishovite	170	80	80	$4 \times 4 \times 6$	$2 \times 2 \times 4$	$30 \times 30 \times 30$
Akimotoite	170	90	120	$4 \times 4 \times 4$	$4 \times 4 \times 4$	$20 \times 20 \times 20$
Lime	80	80	120	$4 \times 4 \times 4$	$4 \times 4 \times 4$	$30 \times 30 \times 30$
Corundum	130	130	130	$4 \times 4 \times 4$	$4 \times 4 \times 4$	$20 \times 20 \times 20$

Results: equation of state at 300K (V_0/Z)



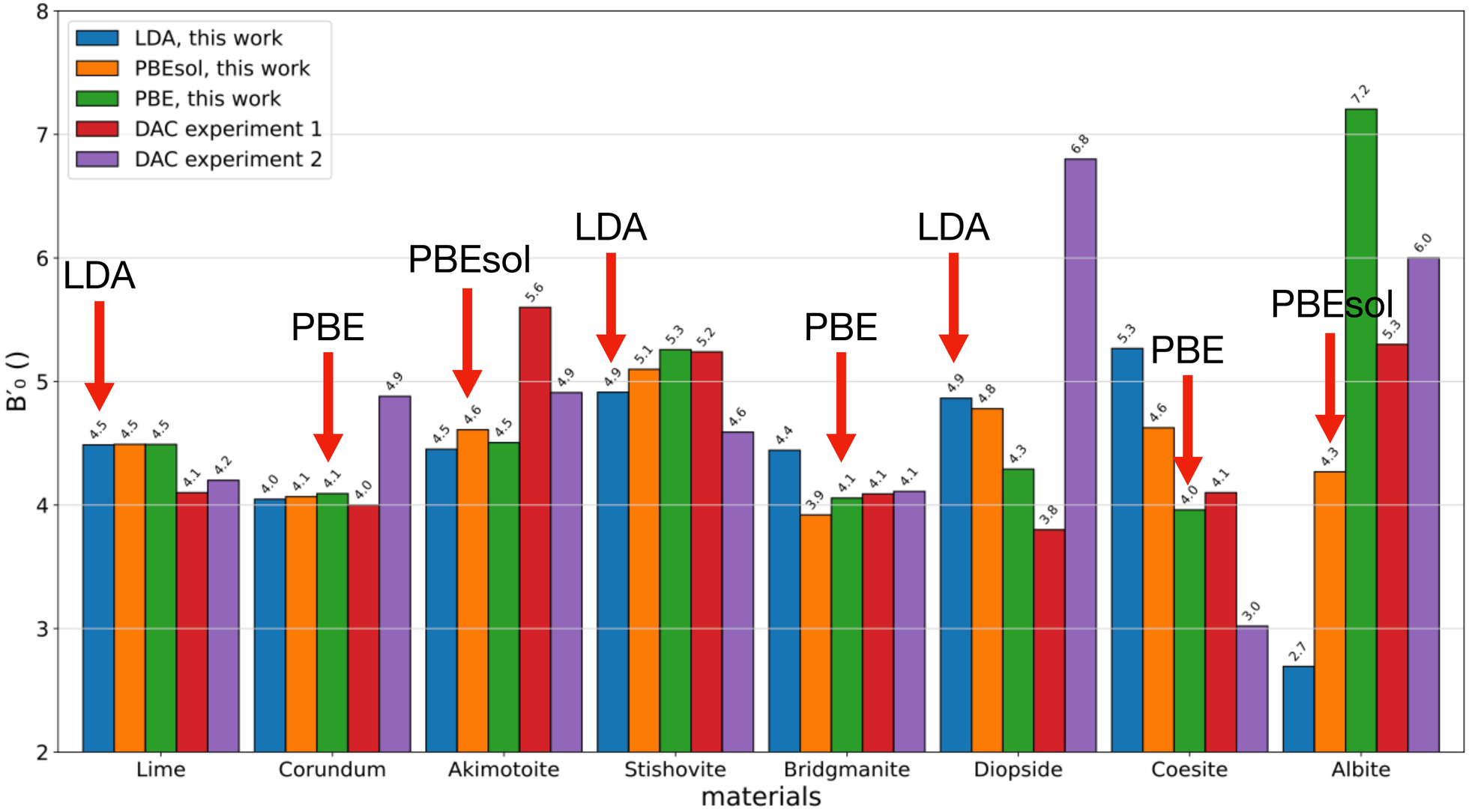
Comparisons between calculated and experimental parameters V_0 at 300 K for the investigated materials, fitted by third-order Birch–Murnaghan equations of state.

Results: equation of state at 300K (B_0)



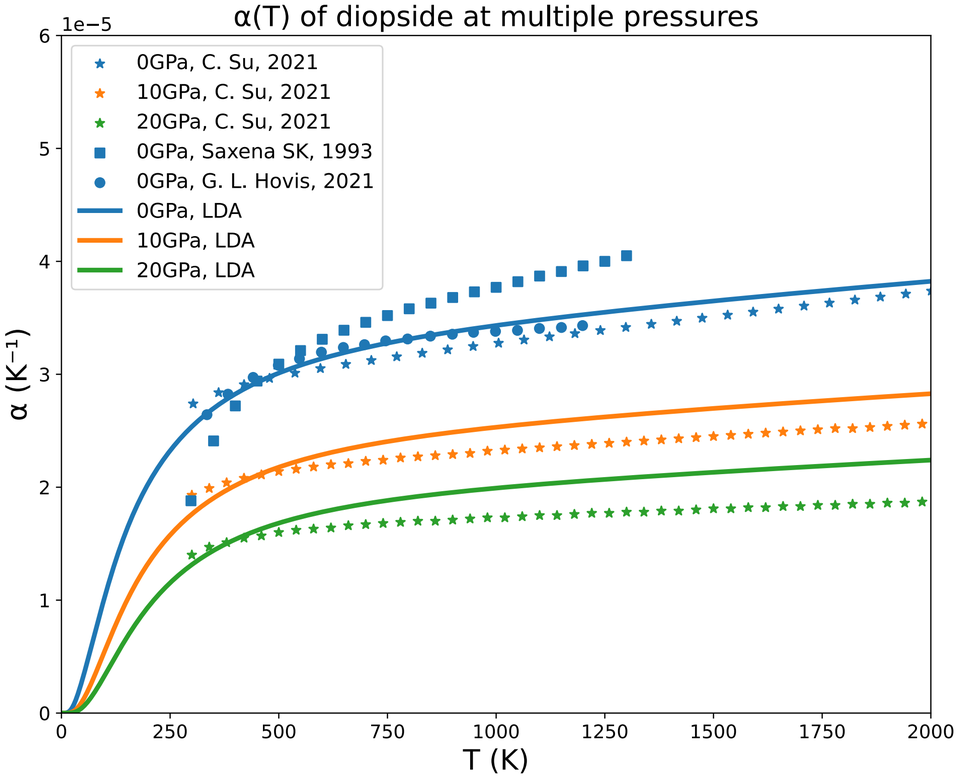
Comparisons between calculated and experimental parameters B_0 at 300 K for the investigated materials, fitted by third-order Birch–Murnaghan equations of state.

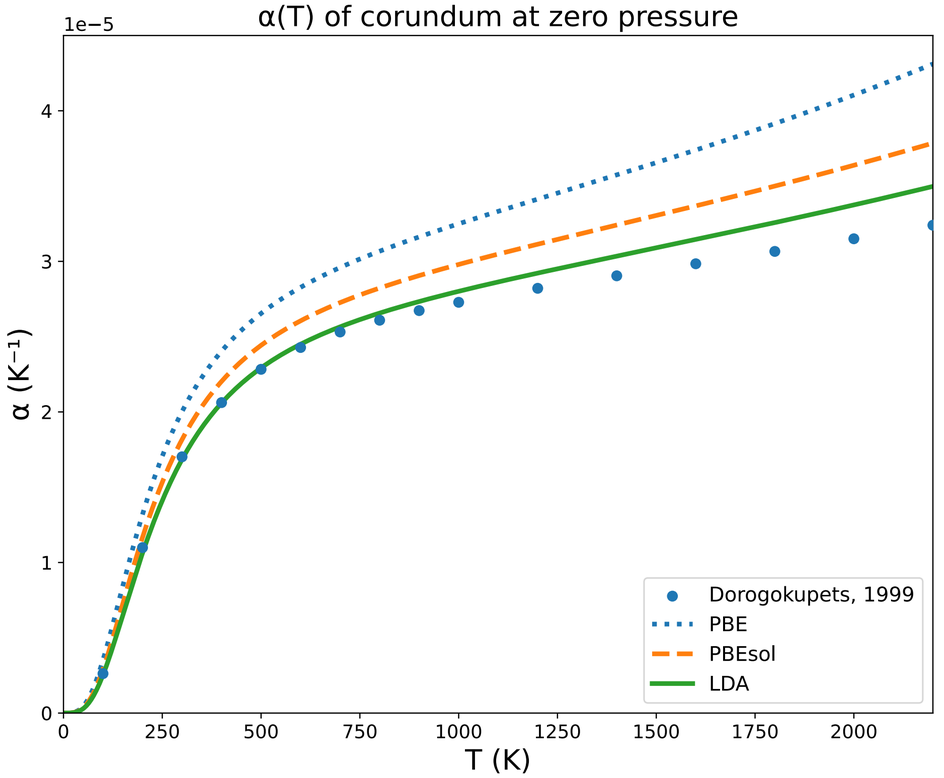
Results: equation of state at 300K (B_0')



Comparisons between calculated and experimental parameters B'$_0$ at 300 K for the investigated materials, fitted by third-order Birch–Murnaghan equations of state.

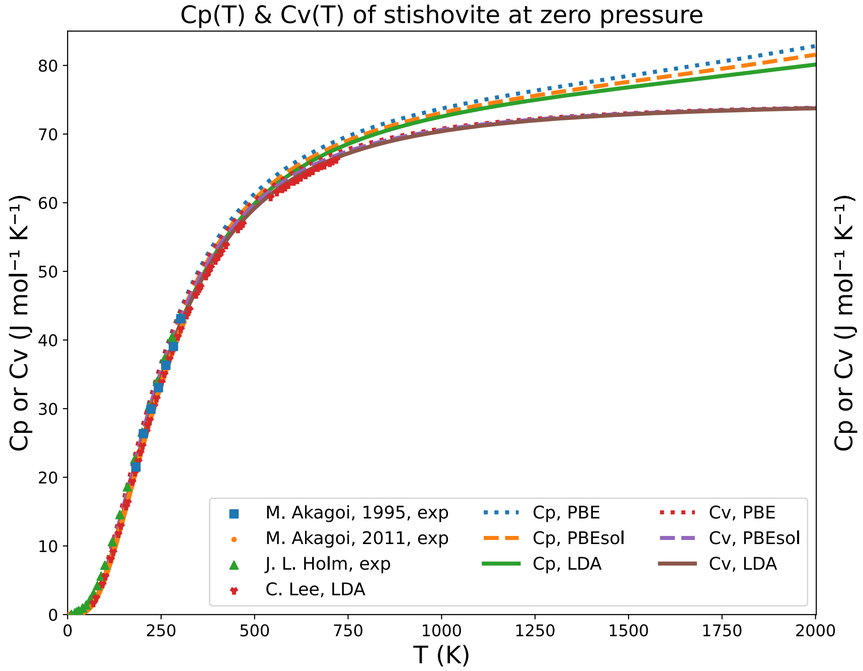
Results: thermal expansion coefficient

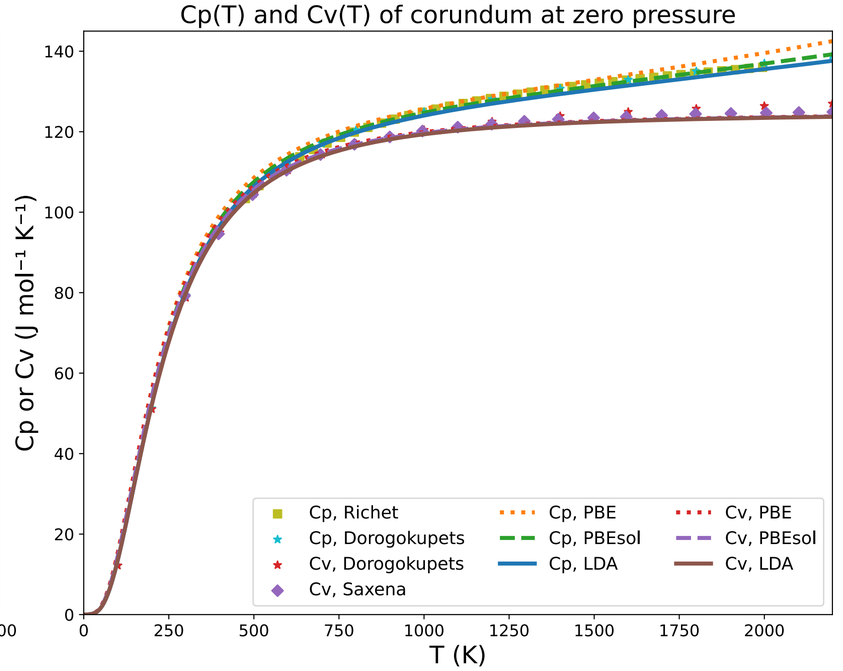


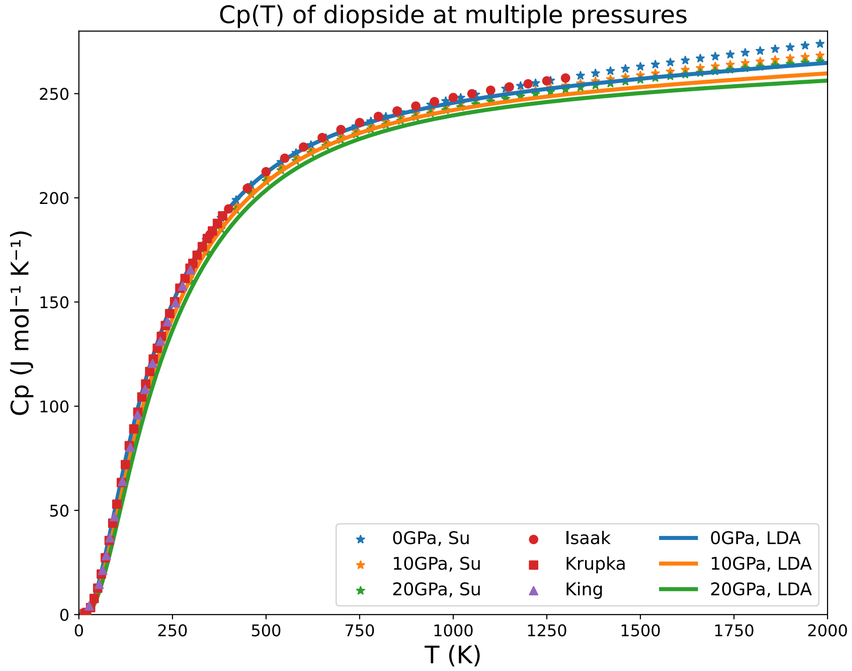


- C. Su *et al.*, *Mineral-basel*. **11**, 1322 (2021).
- D. G. Isaak, I. Ohno, P. C. Lee, Phys Chem Miner. 32, 691–699 (2006).
- G. L. Hovis et al., Am Mineral. 106, 883–899 (2021).
- Saxena SK, Chatterjee N, Fei Y, Shen G (1993) Thermodynamic data on oxides and silicates. Springer, Berlin Heidelberg New York, pp 168–169

Results: specific heat







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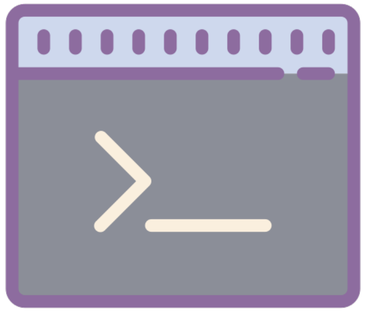
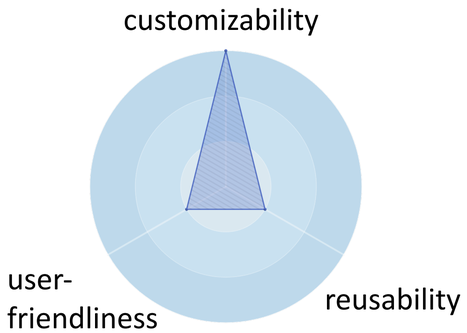
- C. Su *et al.*, *Mineral-basel*. **11**, 1322 (2021).
- D. G. Isaak, I. Ohno, P. C. Lee, Phys Chem Miner. 32, 691–699 (2006).
- G. L. Hovis et al., Am Mineral. 106, 883–899 (2021).
- Saxena SK, Chatterjee N, Fei Y, Shen G (1993) Thermodynamic data on oxides and silicates. Springer, Berlin Heidelberg New York, pp 168–169

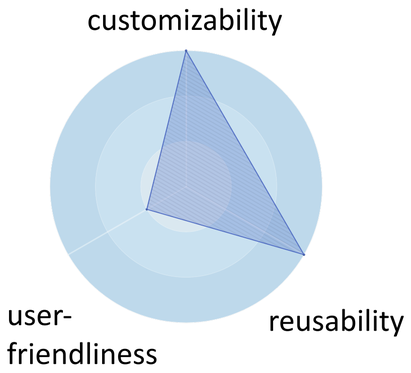
`express` implements 3 common user interfaces

terminal✅

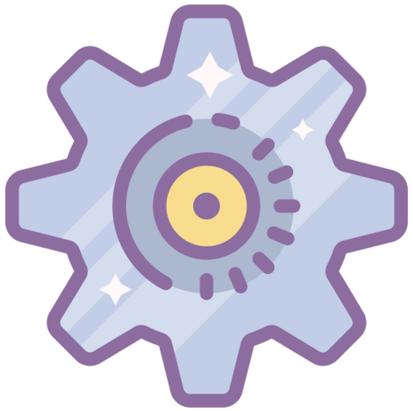


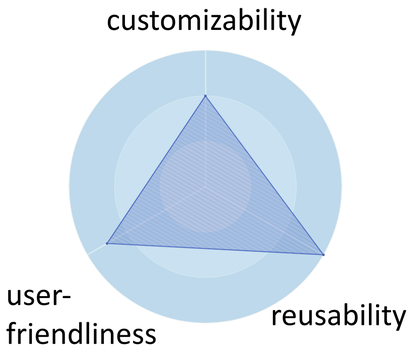


script✅

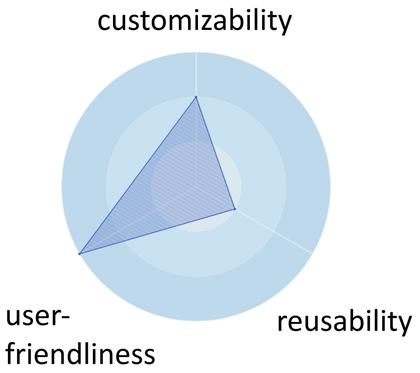


config file✅

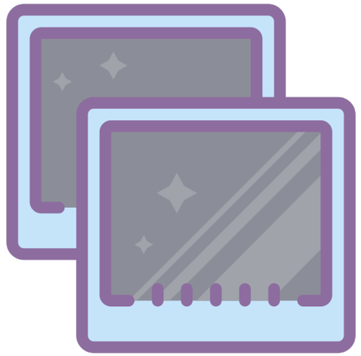




web/app❌



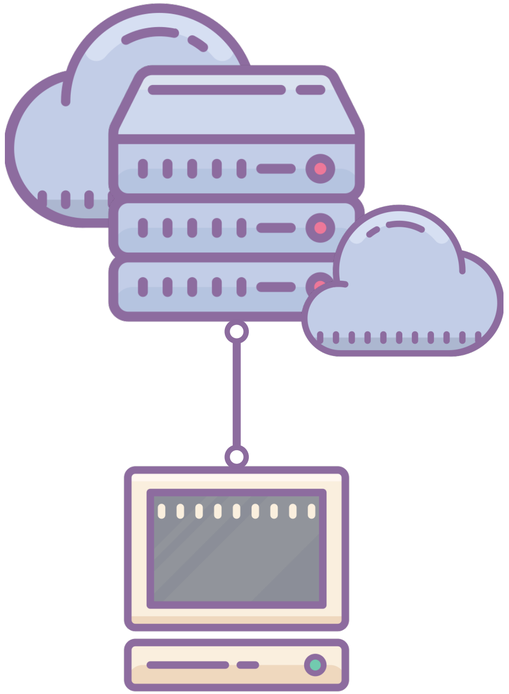
Code deployment on different environments



virtual machines or
(Docker) containers

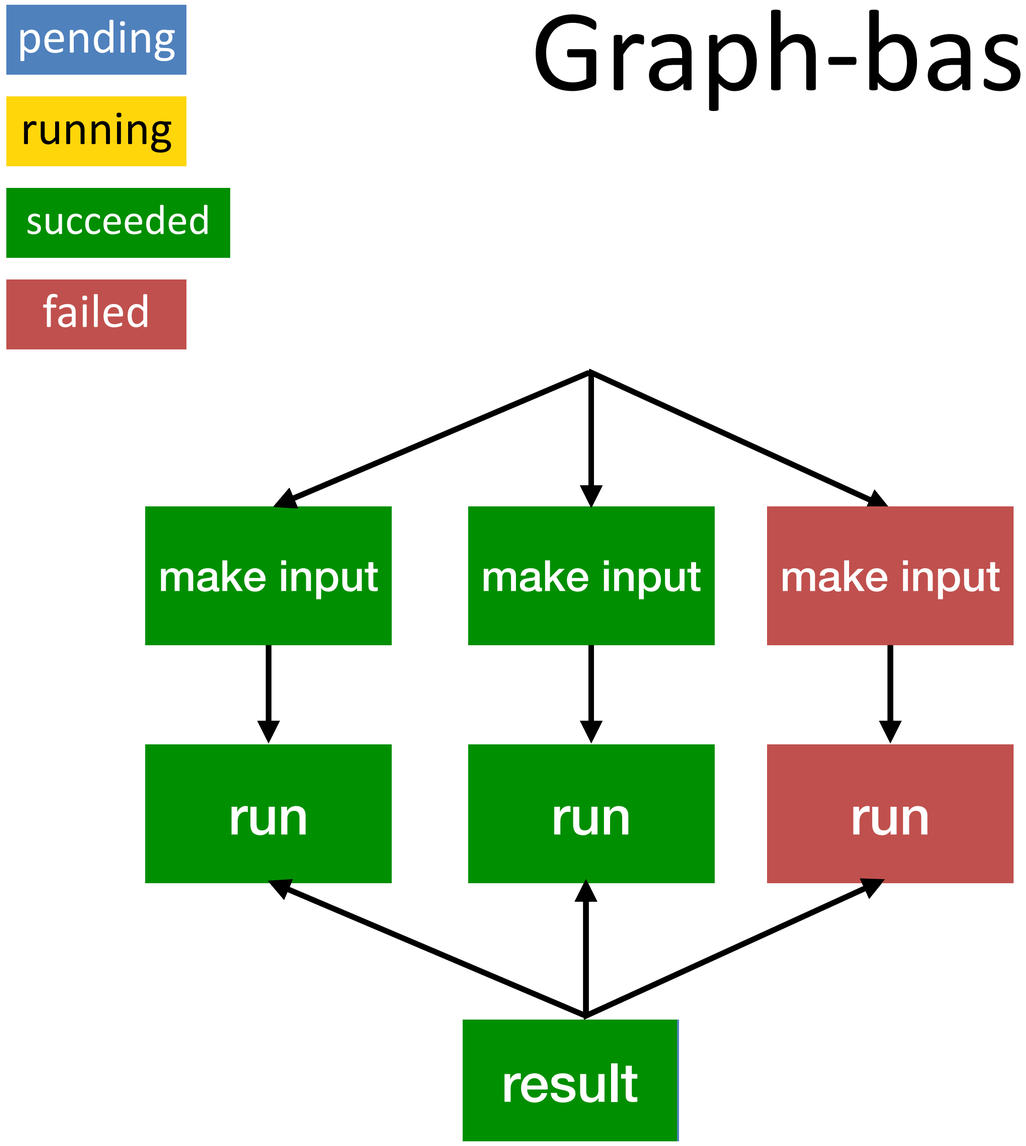
local PCs

remote servers



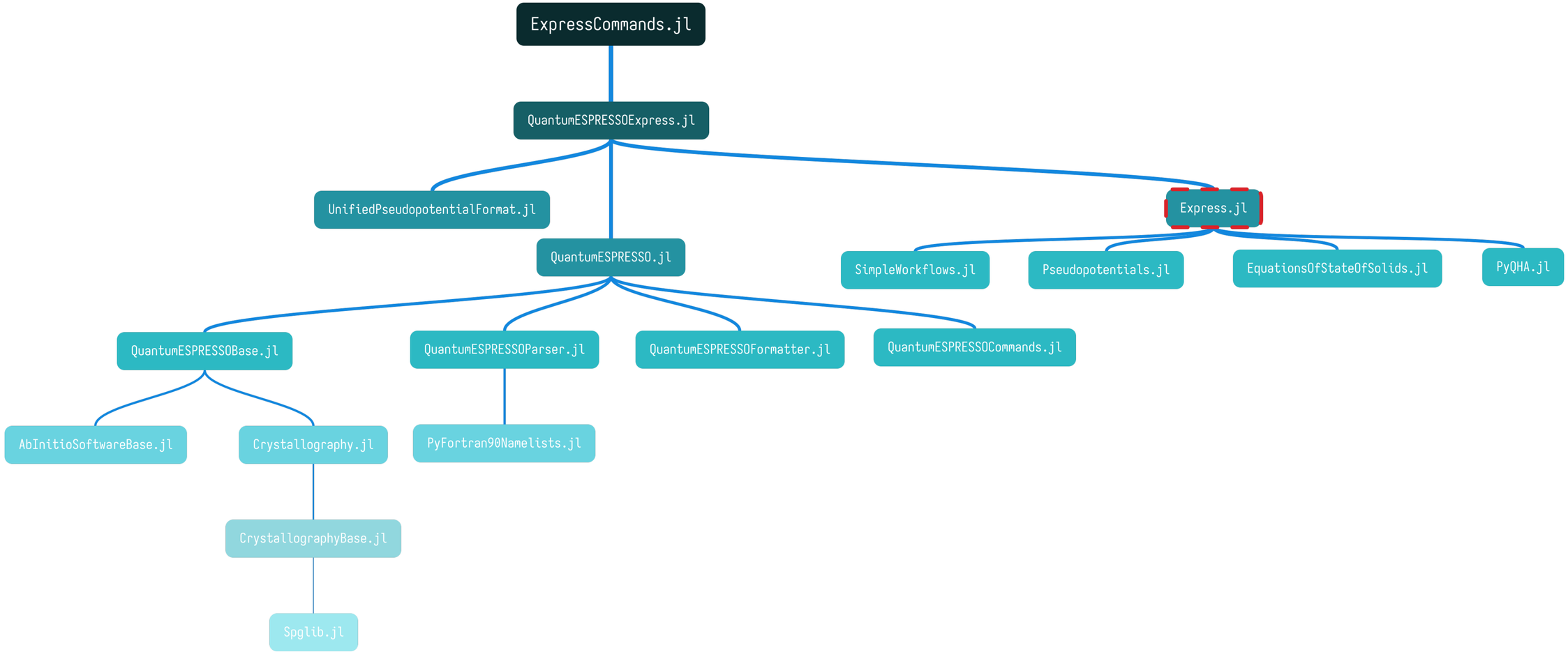
multiple environments

Graph-based workflow model



- Each action (make input, run QE, read output, etc.) is a `Node` in the DAG representation of the workflow
- Each `Node` tracks the status and other metadata (time, result, etc.) of the action
- The status of the workflow is saved to a file while running, interrupted/failed actions can be rerun after restarting/fixing
- Workflows can be stored in a database for future reference

Components of the `express` project



EOS workflow input files

- A config file
  - Desired pressures for optimization
  - A trial equation of state
  - Computational settings
- A QE template input for SCF

```yaml
recipe: eos
cli:
  mpi:
    np: 16
  pw:
    path: ~/bin/pw.x
template: template.in
save:
  status: status.jls
fixed:
  pressures:
    unit: GPa
    values:
      - -5
      - -2
      - 0
      - 5
      - 10
      - 15
      - 17
      - 20
trial_eos:
  type: bm3
  values:
    - 300.44 bohr^3
    - 74.88 GPa
    - 4.82
```

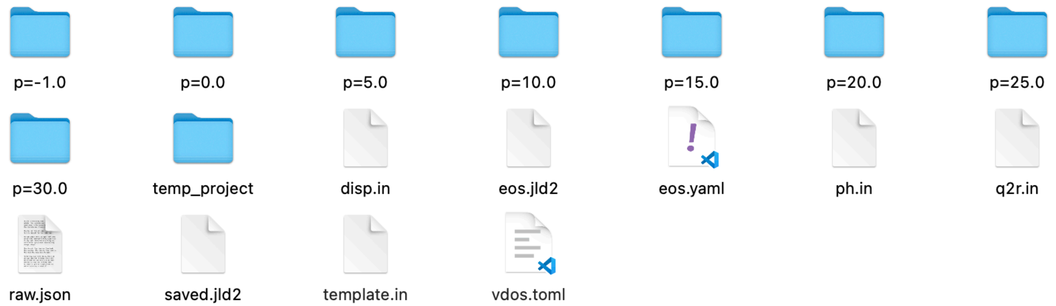
```
&control
calculation='scf'
pseudo_dir  = './pseudo'
prefix='Ge'
outdir   = './'
/
&system
ibrav=2
celldm(1)=7.957636
nat=2
ntyp=1
ecutwfc = 55
/
&electrons
conv_thr=1.0d-10
/
ATOMIC_SPECIES
Ge    72.64    Ge.pz-dn-kjpaw_psl.0.2.2.UPF

ATOMIC_POSITIONS (crystal)
Ge    0.00000    0.00000    0.00000
Ge    0.75000    0.75000    0.75000
K_POINTS automatic
6 6 6 1 1 1
```

EOS workflow output files

- SCF and vc-relax inputs and outputs for each pressure
- Fitted equations of state
- $E(V)$ raw data for SCF and vc-relax
- Tracked running status of each job in the workflow

Before

After



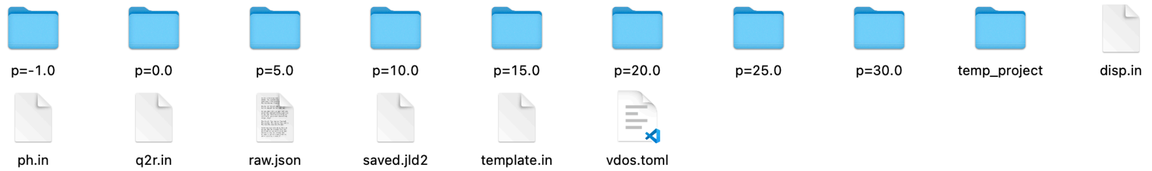
Phonon workflow input files

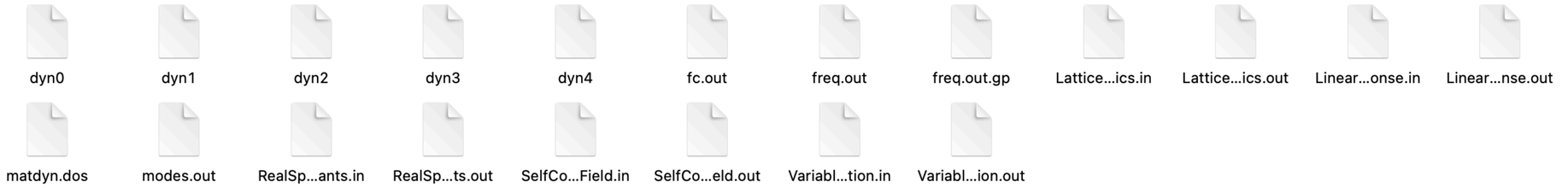
- A config file
  - Desired pressures
  - Computational settings
- QE template input files for SCF, DFPT, force constant calculations, phonon dispersion calculations

```yaml
recipe: vdos
cli:
  mpi:
    np: 16
template:
  scf: ../examples/Ge/template.in
  dfpt: ../examples/Ge/ph.in
  q2r: ../examples/Ge/q2r.in
  disp: ../examples/Ge/disp.in
save:
  status: status.jld2
fixed:
  pressures:
    unit: GPa
    values:
      - -5
      - -2
      - 0
      - 5
      - 10
      - 15
      - 17
      - 20
```

Phonon workflow output files

- SCF, DFPT, force constant calculations', phonon dispersion calculations' inputs and outputs for each pressure
- Tracked running status of each job in the workflow





QHA workflow input files

- QE output of phonon frequencies from the phonon workflow
- Q-points
- Static $E(V)$ relations on each desired pressure

```
comment: Si calculated by Quantum ESPRESSO
formula_unit_number: 2
frequency_files:
  - ../examples/silicon/V+5.freq
  - ../examples/silicon/V+4.freq
  - ../examples/silicon/V+3.freq
  - ../examples/silicon/V+2.freq
  - ../examples/silicon/V+1.freq
  - ../examples/silicon/V0.freq
  - ../examples/silicon/V-1.freq
  - ../examples/silicon/V-2.freq
  - ../examples/silicon/V-3.freq
  - ../examples/silicon/V-4.freq
  - ../examples/silicon/V-5.freq
```

```
 0.0000000   0.0000000   0.0000000   0.0092593
-0.1666667   0.1666667  -0.1666667   0.0740741
-0.3333333   0.3333333  -0.3333333   0.0740741
 0.5000000  -0.5000000   0.5000000   0.0370370
 0.0000000   0.3333333   0.0000000   0.0555556
-0.1666667   0.5000000  -0.1666667   0.2222222
 0.6666667  -0.3333333   0.6666667   0.2222222
 0.5000000  -0.1666667   0.5000000   0.2222222
 0.3333333   0.0000000   0.3333333   0.1111111
 0.0000000   0.6666667   0.0000000   0.0555556
 0.8333333  -0.1666667   0.8333333   0.2222222
 0.6666667  -0.0000000   0.6666667   0.1111111
 0.0000000  -1.0000000   0.0000000   0.0277778
 0.6666667  -0.3333333   1.0000000   0.2222222
 0.5000000  -0.1666667   0.8333333   0.2222222
-0.3333333  -1.0000000   0.0000000   0.1111111
```

```
P=     -93.46  V=     320.5259        E=     -15.72569834
P=     -80.32  V=     311.4549        E=     -15.73098435
P=     -64.79  V=     302.5568        E=     -15.73530702
P=     -46.61  V=     293.8297        E=     -15.73854690
P=     -25.53  V=     285.2721        E=     -15.74057452
P=      -1.21  V=     276.8823        E=     -15.74126580
P=      26.68  V=     268.6586        E=     -15.74048328
P=      58.52  V=     260.5994        E=     -15.73807360
P=      94.69  V=     252.7030        E=     -15.73387649
P=     135.65  V=     244.9677        E=     -15.72772377
P=     181.94  V=     237.3920        E=     -15.71945542
```

QHA workflow output files

- Output
- Input for the qha code
- Thermodynamic properties as functions of (T, V) and (T, P)
- Plots of these thermodynamic properties

Slurm commands

- `srun --partition=debug  --pty --account=col146 --nodes=1 --ntasks-per-node=112 --mem=128G -t 00:30:00 --wait=0 --export=ALL zsh`
- `squeue --me`

Summary

Therefore, we made a software that

- is easy to use. Users can rely on these highly-customizable workflows with different *ab initio* software while writing little to no code.

- can calculate multiple thermodynamic and thermoelastic properties on various materials with *ab initio* methods.

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