Implementation of the Strain Perturbation in ABINIT

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Overview

- **Goal**: Direct calculation of the elastic and piezoelectric tensors and related quantities
- Strain and the Abinit reduced-coordinate formulation
- Brief review of density functional perturbation theory
- Response function (RF) code organization
- Development process design
- Special issues: nonlocal pseudopotentials, symmetry, non-linear core corrections, cutoff smoothing, metals
- Using: new input and output
- Atom coordinate relaxation and anaddb post processing
- Future development issues
- (Appendix)
Strain tensor $\eta_{\alpha\beta}$ as a perturbation

- Strain really only changes the positions of the atomic (pseudo)potentials,

$$V_{ext}(\mathbf{r}) = \sum_{R} \sum_{\tau}^{\text{cell}} V_{\tau}(\mathbf{r} - \mathbf{\tau} - \mathbf{R}) \rightarrow V_{ext}(\mathbf{r}) = \sum_{R} \sum_{\tau}^{\text{cell}} V_{\tau}[\mathbf{r} - (1 + \eta) \cdot \mathbf{\tau} - (1 + \eta) \cdot \mathbf{R}].$$

- However, this causes unique problems for perturbations expansions:
  - Viewed in terms of the infinite lattice, the strain perturbation can never be small.
  - From the point of view of a single unit cell, strain changes the periodic boundary conditions, so wave functions of the strained lattice cannot be expanded in terms of those of the unstrained lattice.

- Strain appears to be qualitatively different from other perturbations such as periodicity-preserving atomic displacements.
Strain tensor \( \eta_{\alpha\beta} \) as a perturbation, continued

- **Existing formulation\(^{(1)}\)**
  - Introduce fictitious strained self-consistent Hamiltonian obtained by a scale transformation of the unstrained Hamiltonian,
    \[
    \tilde{H}_{SCF}^\eta (\mathbf{r}, \nabla) = H_{SCF} \left[ (1+\eta)^{-1} \cdot \mathbf{r}, (1+\eta) \cdot \nabla \right]
    \]
  - \( \tilde{H}_{SCF}^\eta \) obeys the same boundary conditions as the strained Hamiltonian
  - \( \tilde{H}_{SCF}^\eta \) has the same spectrum unstrained Hamiltonian, and a simply related electron density \( \tilde{n}^\eta(\mathbf{r}) \)
  - Energy difference between unstrained crystal and fictitious strained crystal described by \( \tilde{H}_{SCF}^\eta \) is easily obtained

- **Problem:** Hartree and XC potentials of \( \tilde{H}_{SCF}^\eta \) are not those generated by \( \tilde{n}^\eta(\mathbf{r}) \) so \( \tilde{H}_{SCF}^\eta \) is not a genuine Kohn-Sham Hamiltonian
  - Must introduce modified external potential \( \tilde{V}_{ext}^\eta \) to compensate
  - Then use DFPT treating \( V_{ext}^\eta - \tilde{V}_{ext}^\eta \) as the perturbation

- Complex two-step process apparently changes the structure of DPFT from that for other perturbations

Abinit reduced coordinate (~) formulation

• Every lattice, unstrained or strained, is a unit cube in reduced coordinates.
  – Primitive real and reciprocal lattice vectors define the transformations:

\[ X_\alpha = \sum_i R^{p}_{\alpha i} \tilde{X}_i , \quad K_\alpha \equiv (k_\alpha + G_\alpha) = \sum_i G^{p}_{\alpha i} \tilde{K}_i , \quad \sum_\alpha R^{p}_{\alpha i} G^{p}_{\alpha j} = 2\pi \delta_{ij} \]

  – Cartesian indices \( \alpha, \beta, \cdots = 1,3 \) and reduced indices \( i, j, \cdots = 1,3 \)

• Every term in the DFT functional can be expressed in terms of dot products and the unit cell volume \( \Omega \).
  – Dot products and \( \Omega \) in reduced coordinates are computed with metric tensors,

\[ X' \cdot X = \sum_{ij} \tilde{X}'_i \Xi_{ij} \tilde{X}'_j , \quad K' \cdot K = \sum_{ij} \tilde{K}'_i \Upsilon_{ij} \tilde{K}'_j , \quad \Omega = (\det[\Xi_{ij}])^{1/2} \]

• Strain is now a “simple” parameter of a density functional whose wave functions have invariant boundary conditions.
Abinit reduced coordinate (~) formulation

- Strain derivatives act **only** on the metric tensors,
  \[
  \Xi_{ij}^{(\alpha\beta)} = \frac{\partial \Xi_{ij}}{\partial \eta_{\alpha\beta}} = R_{\alpha i}^P R_{\beta j}^P + R_{\beta i}^P R_{\alpha j}^P, \quad \Gamma_{ij}^{(\alpha\beta)} = -G_{\alpha i}^P G_{\beta j}^P - G_{\beta i}^P G_{\alpha j}^P
  \]

- \( \Xi_{ij}^{(\alpha\beta\gamma\delta)} \) has uniquely simple derivatives for **Cartesian Strains**
  \[
  \frac{\partial^2 \Xi_{ij}}{\partial \eta_{\gamma\delta} \partial \eta_{\alpha\beta}} = \delta_{\alpha\beta\gamma} (R_{\beta i}^P R_{\delta j}^P + R_{\delta i}^P R_{\beta j}^P) + \delta_{\alpha\beta\gamma} (R_{\alpha i}^P R_{\delta j}^P + R_{\delta i}^P R_{\alpha j}^P)
  \]

- **Key decision**: strain will be Cartesian throughout the code
  - Existing perturbations will remain in reduced-coordinates
Stress and strain notation

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- All forms used at various places internally and in output
Density Functional Perturbation Theory

- All quantities are expanded in power series in a DF energy parameter $\lambda$,

$$X(\lambda) = X^{(0)} + \lambda X^{(1)} + \lambda^2 X^{(2)} + \cdots, \quad X = E_{el}, T, V_{ext}, \psi_\alpha(r), n(r), \varepsilon_\alpha, H$$

- Solutions $\psi^{(0)}$ of Kohn-Sham equation minimize the usual DFT functional $E^{(0)}$

$$H^{(0)}|\psi_\alpha^{(0)}\rangle = \varepsilon_\alpha^{(0)}|\psi_\alpha^{(0)}\rangle.$$

- The variational functional for $E^{(2)}$ is minimized by solutions $\psi^{(1)}$ of the self-consistent Sternheimer equation

$$P_c (H^{(0)} - \varepsilon_\alpha^{(0)}) P_c |\psi_\alpha^{(1)}\rangle = -P_c H^{(1)} |\psi_\alpha^{(0)}\rangle,$$

where $P_c$ is the projector on unoccupied states (conduction bands) and

$$H^{(1)} = T^{(1)} + V_{ext}^{(1)} + V_{Hxc}^{(1)}, \quad V_{Hxc}^{(1)} = \frac{\partial}{\partial \lambda} \frac{\delta E_{Hxc}}{\delta n(r)} \bigg|_{n^{(0)}} + \int \frac{\delta^2 E_{Hxc}}{\delta n(r) \delta n(r')} n^{(1)}(r') dr',$$

$$n^{(1)}(r) = \sum_{\alpha}^{occ} [\psi^{*(1)}_\alpha(r) \psi^{(0)}_\alpha(r) + \psi^{*(0)}_\alpha(r) \psi^{*(1)}_\alpha(r)].$$
DFPT for elastic and piezoelectric tensors

- Mixed 2nd derivatives of the energy with respect to two perturbations are needed.
  - By the “2n+1” theorem, these only require one set of 1st order wave functions,
    \[
    E_{el}^{(λ_1λ_2)} = \sum_α^{occ} \langle ψ_α^{(λ_2)} | (T^{(λ_1)} + V_{ext}^{(λ_1)} + H_{Hxc0}^{(λ_1)}) | ψ_α^{(0)} \rangle 
    + \sum_α^{occ} \langle ψ_α^{(0)} | (T^{(λ_1λ_2)} + V_{ext}^{(λ_1λ_2)}) | ψ_α^{(0)} \rangle + \frac{1}{2} \frac{\partial^2 E_{Hxc}}{\partial λ_1 \partial λ_2} |_{n^{(0)}} ,
    \]

- Including atomic relaxation, we need
  - Clamped-atom elastic tensor ---------- \( \partial^2 E_{el} / \partial η_{αβ} \partial η_{γδ} \)
  - Internal strain tensor ------------------- \( \partial^2 E_{el} / \partial η_{αβ} \partial \tilde{τ}_j \)
  - Interatomic force constants ---------- \( \partial^2 E_{el} / \partial \tilde{τ}_i \partial \tilde{τ}_j \)
  - Clamped-atom piezoelectric tensor ---- \( \partial^2 E_{el} / \partial η_{αβ} \partial \tilde{E}_j \)
  - Born effective charges ------------------ \( \partial^2 E_{el} / \partial \tilde{τ}_i \partial \tilde{E}_j \)

Available

Available
Response function code organization

\[ \langle 0 | H^{(2)} | 0 \rangle \]

\[ \langle K | H^{(1)} | 0 \rangle \]

Sternheimer Eq.,

\[ \langle 1' | H^{(1)} | 0 \rangle \]
Design of development process

- Four stages based on RF code organization and degree of complexity
  - First $\langle K|H^{(1)}|0\rangle$, second Sternheimer, third $\langle 0|H^{(2)}|0\rangle$, and fourth $\langle 1'|H^{(3)}|0\rangle$

- Stage-by-stage and term-by-term validation based on existing GS first derivatives of the total energy (1DTE’s)

- First stage
  - Re-compute stress as $\langle 0|H^{(1)}|0\rangle = \sum_k \langle 0|K\rangle\langle K|H^{(1)}|0\rangle$
  - Compare term-by-term to stress breakdown available in GS calculation:

| stress: component | 1 of hartree stress is | -8.625241635590E-04 |
| stress: component | 2 of hartree stress is | -7.368896556922E-04 |
| stress: component | 1 of loc psp stress is | 2.656792257661E-03 |
| stress: component | 2 of loc psp stress is | 2.166978270656E-03 |
| stress: component | 1 of xc stress is | 4.902613744139E-03 |
| stress: component | 2 of xc stress is | 4.902613744139E-03 |
| stress: ii (diagonal) part is | -7.753477394392E-03 |
| stress: component | 1 of kinetic stress is | -5.477053634248E-03 |
| stress: component | 2 of kinetic stress is | -5.272489903492E-03 |
| stress: component | 1 of nonlocal ps stress is | 2.396391029219E-03 |
| stress: component | 2 of nonlocal ps stress is | 1.907769135572E-03 |
| stress: component | 1 of Ewald energ stress is | 5.707853334522E-03 |
| stress: component | 2 of Ewald energ stress is | 6.846039389167E-03 |
| stress: component | 1 of core xc stress is | -1.789801472019E-03 |
| stress: component | 2 of core xc stress is | -1.911589314962E-03 |
Design of development process (continued)

- Second through fourth stage – numerical derivatives of GS quantities
  - “Five-point” strain first derivatives of GS quantities (symmetric shear strains)
  - Strain increments small enough to keep complete $\{\mathbf{K}\}$ set invariant
  - Second derivatives of total energy (2DTE’s) from numerical derivatives of 1DTE’s (e.g., stress)
    - Extreme convergence of self-consistency required, but not of $k$’s or cutoffs

- Second stage – Sternheimer
  - Convergence of self-consistency loop
  - Ensure variational part of RF 2DTE’s decreases with convergence
  - First-order density $n^{(1)}$ validated by comparison with numerical $n^{(0)}$ derivatives

- Second stage – validation of variational RF 2DTE’s
  - Non-variational part $\langle 0|H^{(2)}|0 \rangle$ not yet available
  - Compute numerical 2DTE’s as above with converged GS wave functions for strained lattices
  - Subtract numerical 2DTE’s with strained lattices but unstrained (“frozen”) GS wave functions

- So far, we are only dealing with “diagonal” 2DTE’s
Third stage – \( \langle 0 | H^{(2)} | 0 \rangle \):

\[
E^{(\lambda_1, \lambda_2)}_{\text{non-var}} = \sum_{\alpha, \alpha'}^{\text{occ}} \langle \psi^{(0)}_\alpha | (T^{(\lambda_1, \lambda_2)} + V_{\text{ext}}^{(\lambda_1, \lambda_2)}) \psi^{(0)}_\alpha \rangle + \frac{1}{2} \left[ \left. \frac{\partial^2 E_{\text{Hxc}}}{\partial \lambda_1 \partial \lambda_2} \right|_{n^{(0)}} \right]
\]

- Validate term-by-term with “frozen wave function” numerical strain derivatives of stress components
- Diagonal and off-diagonal 2DTE’s
- Numerical strain derivatives of forces for internal strain mixed 2DTE’s
- Frozen wf strain derivatives of the electric polarization are zero, so there is no contribution to piezoelectric tensor from these terms

Note that the numerical derivatives of stress \( \sigma \) need \( \Omega \) factor for 2DTE comparison

\[
\frac{\partial^2 E_{\text{el}}}{\partial \eta_{\alpha \beta} \partial \eta_{\gamma \delta}} = \frac{\partial}{\partial \eta_{\alpha \beta}} \left( \Omega \sigma_{\gamma \delta} \right)
\]
Design of development process (continued)

- Fourth stage – 
  \[ E_{\text{non-stat}}^{(\lambda_1, \lambda_2)} = \sum_{\alpha}^{\text{occ}} \langle \psi_{\alpha}^{(\lambda_2)} | (T^{(\lambda_1)} + V_{\text{ext}}^{(\lambda_1)} + H_{Hxc0}^{(\lambda_1)}) | \psi_{\alpha}^{(0)} \rangle \]
  - Use strain-perturbation wave functions \( \psi_{\alpha}^{(\lambda_2)} \)
  - \( \lambda_1 \) is Cartesian strain or reduced atomic displacement

- Electric field is special case – 
  \[ \frac{\partial^2 E_{el}}{\partial \tilde{\mathcal{E}}_j \partial \eta_{\alpha\beta}} = \frac{2\Omega}{(2\pi)^3} \int_{\text{BZ}} \sum_{m}^{\text{occ}} \langle i \psi_{km}^{(\tilde{k}_j)} | \psi_{km}^{(\eta_{\alpha\beta})} \rangle dk \]
  - Field and \( d/dk \) first-order wave function in reduced coordinates

- Validate using numerical strain derivatives of GS stresses, forces, and polarization
  - Use converged strained wave functions
  - No subtractions since non-variational contributions are already validated
  - For polarization, numerical derivatives have to be corrected to give “proper” piezoelectric tensor (see Infos/theory/lr.pdf)
  - Need to use finite-difference \( d/dk \) wf’s in RF calculation for accurate comparison
# Subroutines for strain perturbation (53)

## Modified routines

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## Utility

\[
\langle K | H^{(1)} | 0 \rangle \quad \langle 1' | H^{(1)} | 0 \rangle \quad \langle 0 | H^{(2)} | 0 \rangle
\]

**Mnemonics**

- **str** – strain, **eltfr** – elastic tensor frozen
- **istr** – internal strain, **cont** – contraction
Nonlocal pseudopotentials in Abinit

- Most mathematically complex object for strain derivatives
- Reduced wave vector matrix elements have the form

\[
\langle \tilde{K}' | V_{NL} | \tilde{K} \rangle = \frac{1}{\Omega} \sum_{\kappa \ell} e^{2\pi i \tilde{K}' \cdot \tilde{\tau}_\kappa} f_{\kappa \ell} \left( \sum_{ij} Y_{ij} \tilde{K}'_i \tilde{K}'_j \right) \times \\
\langle \mathcal{D}_\ell \left( \sum_{ij} Y_{ij} \tilde{K}'_i \tilde{K}'_j, \sum_{ij} Y_{ij} \tilde{K}'_i \tilde{K}'_j, \sum_{ij} Y_{ij} \tilde{K}'_i \tilde{K}'_j \right) e^{-2\pi i \tilde{K} \cdot \tilde{\tau}_\kappa} f_{\kappa \ell} \left( \sum_{ij} Y_{ij} \tilde{K}_i \tilde{K}_j \right) \\
- \mathcal{D}_\ell \text{ modified Legendre polynomials, } f_{\kappa \ell} \text{ psp form factors, } \tilde{\tau}_\kappa \text{ reduced atom coordinates} \\
- All arguments are dot products expressed with metric tensors
- Psp's act on wave functions (in `opernl*.f`) by summing wave function coefficients \( c_{aK} \) times a set of tensor products of reduced \( \tilde{K} \) components,

\[
T_{\ell m} (\tilde{K}) = \tilde{K}_1 I_T(1, \ell, m) \tilde{K}_2 I_T(2, \ell, m) \tilde{K}_3 I_T(1, \ell, m) - I_T(2, \ell, m)
\]

- \( I_T(i, \ell, m) \) are index arrays
- \( T_{\ell m} (\tilde{K}) \) (created in `mkffkq.f`) are analogous to spherical harmonics

(1) D. C. Allan (unpublished, ~ 1987)
Nonlocal pseudopotential strain derivatives

- Mathematica programs created to do symbolic differentiation and extract coefficients coupling pairs of “input” ($\tilde{K}$) and “output” ($\tilde{K}'$) tensors
- Coefficients are polynomials in $\gamma_{ij}, \gamma_{ij}^{(\alpha\beta)}, \gamma_{ij}^{(\gamma\delta)}, \gamma_{ij}^{(\alpha\beta\gamma\delta)}$
- SED and C programs turn Mathematica results into useful Fortran 90
  - Example from contstr24.f

```fortran
cm(6, 10) = (gm(1, 3)**2 * (270 * dgm01(2, 3) * dgm10(1, 1) + 540 * dgm01(1, 3) * dgm10(1, 2) * dgm01(1, 1) * dgm10(1, 2)) &
& + gm(3, 3) * (-108 * gm(1, 2) * (dgm01(1, 3) * dgm10(1, 1) + dgm01(1, 1) * dgm10(1, 2)) &
& + gm(1, 1) * (-54 * dgm01(2, 3) * dgm10(1, 1) - 108 * dgm01(1, 3) * dgm10(1, 2) &
& - 108 * dgm01(1, 2) * dgm10(1, 3) - 108 * gm(1, 1) * dgm10(1, 3)) + gm(2, 3) &
& + dgm01(3, 3) * dgm10(1, 1) + dgm01(1, 1) * dgm10(3, 3)) + 270 * gm(1, 3) ** 2 * d2gm(1, 1) &
& + gm(3, 3) * (-108 * dgm01(1, 1) * dgm10(1, 1) - 54 * gm(1, 1) * d2gm(1, 1)) + 180 * gm(1, 3) &
& * 3 * d2gm(1, 2) + gm(1, 3) * (-108 * gm(1, 2) * (dgm01(3, 3) * dgm10(1, 1) + dgm01(1, 1) &
& * dgm10(3, 3)) + gm(1, 1) * (dgm01(3, 3) * dgm10(1, 2) + dgm01(1, 2) * dgm10(3, 3)) &
& + gm(3, 3) * (-216 * dgm01(1, 2) * dgm10(1, 1) - 216 * dgm01(1, 1) * dgm10(1, 2) &
& - 108 * gm(1, 2) * d2gm(1, 1) - 108 * gm(1, 1) * d2gm(1, 2))) / 36.0
```

- Here $gm(i, j), dgm*(i, j), d2gm(i, j)$ are $\gamma_{ij}$, etc.
- Many 1000’s of lines of infrequently executed code in cont*str*.f and metstr.f
- Evaluation of cm’s is not a major factor in execution time
Symmetry with the strain perturbation

- The reduced-zone $\mathbf{k}$ sample determined for (space group / strain) is used for $\langle \mathbf{K} | H^{(i)} | 0 \rangle$, *Sternheimer*, and $\langle \mathbf{1}' | H^{(i)} | 0 \rangle$
  - The full-zone sample specified in input data must have the full space group symmetry (enforced by test).
- Loop on $(\text{ipert1, idir1})$ for 1st-order wave functions restricted by input variables $(\text{rfstrs, rfdir})$ but not by symmetry
  - This could be improved, but would have limited impact on performance
- Inner loop on $(\text{ipert2, idir2})$ in $\langle \mathbf{1}' | H^{(i)} | 0 \rangle$ calculations is carried over all strain and atomic displacement terms
  - Piezoelectric contribution is computed if $d/dk$_wf’s are available
- All $\langle 0 | H^{(2)} | 0 \rangle$ strain and internal-strain tensor elements are computed, using the full zone $\mathbf{k}$ sample
  - It is more efficient here to keep loops on strains and displacements inside routines like nonlop.f
  - The reduced zone for pairs of perturbations would seldom be reduced much anyway
XC non-linear core correction

- On the reduced real-space grid, electron charge depends only on $\Omega^{-1}$
- Model core charge has a detailed dependence on $\Xi_{ij}$
  - Resulting analysis is rather complex
- Core charges must be extremely smooth functions to avoid significant convergence errors
  - Reason: Strain and atomic position derivatives of the xc self-interaction of a single core don’t cancel point-by-point on the grid, but only in the integral
  - Inconsistencies in the treatment of the core charges and their derivatives in some Src_2psp/psp*cc.f routines makes matters worse
Kinetic energy cutoff “smoothing”

- Existing Abinit strategy to smooth energy dependence on lattice parameters in GS calculations
- RF strain derivative calculations do accurately reproduce GS numerical derivatives with non-zero $\text{ecut}_\text{sm}$
- Divergence can produce large shifts in elastic tensor if calculation is not very well converged with respect to $\text{ecut}$
  - Remember, we take two derivatives
  - Perhaps the cutoff function could be improved
Strain perturbation for metals

- Thermal smearing of the Fermi surface must be introduced for stability
- In RF calculations, a band of partially-occupied states around $\varepsilon_F$ is treated by finite-temperature perturbation theory in the Sternheimer solution, and only the completely unoccupied states are found by the conjugate-gradient method \(^{(1)}\)
- For strain, a first-order Fermi energy $\varepsilon_F^{(1)}$ must be introduced \(^{(2)}\)
- $\varepsilon_F^{(1)}$ enters into the Sternheimer self-consistency process
- Convergence can be rather slow
  - Only simple mixing is presently used to iterate $\varepsilon_F^{(1)}$
  - Coupling to the first-order potential iteration through Anderson or CG mixing may help
- Is $\varepsilon_F^{(1)}$ needed for the $Q = 0$ interatomic force constant calculations needed to get the relaxed-atom elastic tensor for metals?

\(^{(2)}\) S. Baroni, S. de Gironcoli, and A. Dal Corso, Rev. Mod. Phys. 73, 515 (2001)
# First dataset : Self-consistent run

# Second dataset : Non-self-consistent run
# for full k point set

# Third dataset : d/dk response calculation
# this section is omitted if
getwfk3 2  # only the elastic tensor is
getden3 1  # wanted
iscf3 -3
rfelfd3 2
rfdir3 1 1 1

# Fourth dataset : phonon, strain, and homogeneous electric field response

diemix4 0.85
diemac4 1.0
getwfk4 2
getddk4 3  # omitted for ELT only
iscf4 3
rfelfd4 3  # omitted for ELT only
rfatpol4 1 2
rfdir4 1 1 1
rfphon4 1
rfstrs4 3  # only this is new for strain

# Common data
# stresses and forces should
# (in general) be relaxed
# beforehand

nqpt 1
qpt 0 0 0
2DTE terms in output file

- Mix of reduced and Cartesian coordinates, also in _DDB output file
  - With `natom = 2`, electric field `pert = 4` and strain `pert = 5, 6`
  - Only a sample of the complete matrix shown

2nd-order matrix (non-cartesian coordinates, masses not included, 
asr not included)
cartesian coordinates for strain terms (1/ucvol factor
for elastic tensor components not included)

<table>
<thead>
<tr>
<th>j1</th>
<th>j2</th>
<th>matrix element</th>
</tr>
</thead>
<tbody>
<tr>
<td>dir</td>
<td>pert</td>
<td>dir</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>2</td>
</tr>
</tbody>
</table>

- Cartesian ELT, PZT, and internal strain are also included in the output
- Detailed breakdown of contributions is given for `prtvol = 10`
Incorporating atomic relaxation

- Implemented as post-processing procedure in anaddb
- Full theoretical discussion in Infos/Theory/lr.pdf
- Basic results:

\[
\tilde{C}_{\alpha\beta,\gamma\delta} = C_{\alpha\beta,\gamma\delta} + \Omega^{-1} \sum_{mn=1}^{natom} \sum_{ij=1}^{3} \Lambda_{mi,\alpha\beta} (K^{-1})_{mi,nj} \Lambda_{nj,\gamma\delta}
\]

\[
\tilde{e}_{\alpha\beta,\gamma} = e_{\alpha\beta,\gamma} + \Omega^{-1} \sum_{mn=1}^{natom} \sum_{ij=1}^{3} \Lambda_{mi,\alpha\beta} (K^{-1})_{mi,nj} Z_{nj,\gamma}
\]

- \(\tilde{C}, C\) physical and clamped-atom elastic tensors
- \(\tilde{e}, e\) physical and clamped-atom piezoelectric tensors
- \(K^{-1}\) pseudo-inverse Q=0 interatomic force constant matrix
- \(\Lambda\) internal-strain “force response” tensor
- \(Z\) Born effective charge matrix
- All in Cartesian coordinates
Input file for anaddb run

```
  dieflag  3  !flag for relaxed-ion dielectric tensor
  elaflag  3  !flag for the elastic tensor
  piezoflag  3  !flag for the piezoelectric tensor
  instrflag  1  !flag for the internal strain tensor

  !the effective charge part
   asr  1
   chneut  1

  !Wavevector list number 1
   nph1l  1
   qph1l  0.0 0.0 0.0 1.0

  !Wave vector list no. 2
   nph2l  1
   qph2l  0.0 0.0 1.0 0.0
```

New flags and/or values in violet

See Test_v4/t61-70 for more examples
New output from anaddb

Elastic Tensor (relaxed ion) (Unit: $10^2$GP, VOIGT notation):

```
1.2499151  0.6699976  0.6835944  0.0022847  -0.0113983  -0.0001512
0.6699976  1.6217899  0.5566207  0.0194005  -0.0055653  -0.0055915
0.6835944  0.5566207  1.5896839  -0.0207927  0.0107924   0.0080825
-0.0113983 -0.0055653  0.0107924  0.0077398   0.7283916   0.0014049
-0.0001512 -0.0055915  0.0080825  -0.0056845  0.0014049  0.7222881
```

Proper piezoelectric constants (relaxed ion) (Unit: c/m^2)

```
0.01714694  0.05107080  -0.00883676
0.00828454  0.03716812  -0.00810176
0.01882065  0.05180658  -0.00576393
-0.03872154 -0.01245206  0.01902693
-0.01424058  0.00757132  -0.00294782
0.01566436  -0.00054740  0.00218470
```

Also in output

- Clamped-ion versions of the above in standard units
- Clamped and relaxed compliance tensors
- “Force-response” and “displacement response” internal strain tensors
- More tensors corresponding to different boundary conditions to be added
Global comparison with numerical derivatives

- Zinc-blende AlP with random distortions so all tensor elements are non-zero.
  - Ground state calculations of stress and polarization with *exquisitely* relaxed atomic coordinates (but unrelaxed stress)
  - Finite-difference $d/dk \psi_a^{(1)}$'s for best consistency with polarization calculations
  - Sample of complete set of tensor elements

<table>
<thead>
<tr>
<th>Elastc Tensor (GPa)</th>
<th>Numerical</th>
<th>DFPT</th>
<th>Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>xx xx</td>
<td>124.991500</td>
<td>124.991500</td>
<td>-1.1E-05</td>
</tr>
<tr>
<td>yy xx</td>
<td>66.999750</td>
<td>66.999760</td>
<td>8.2E-06</td>
</tr>
<tr>
<td>zz xx</td>
<td>68.359440</td>
<td>68.359440</td>
<td>7.0E-07</td>
</tr>
<tr>
<td>yz xx</td>
<td>0.228447</td>
<td>0.228466</td>
<td>1.9E-05</td>
</tr>
<tr>
<td>xz xx</td>
<td>-1.139838</td>
<td>-1.139828</td>
<td>9.6E-06</td>
</tr>
<tr>
<td>xy xx</td>
<td>-0.015028</td>
<td>-0.015117</td>
<td>-9.0E-05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Piezoelectric Tensor (C/m² x 10⁻²)</th>
<th>Numerical</th>
<th>DFPT</th>
<th>Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>xx xx</td>
<td>1.714769</td>
<td>1.714694</td>
<td>-7.5E-05</td>
</tr>
<tr>
<td>y xx</td>
<td>5.107069</td>
<td>5.107080</td>
<td>1.1E-05</td>
</tr>
<tr>
<td>z xx</td>
<td>-0.883676</td>
<td>-0.883767</td>
<td>2.9E-04</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Numerical</th>
<th>DFPT</th>
<th>Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>x yy</td>
<td>0.828569</td>
<td>0.828454</td>
<td>-1.2E-04</td>
</tr>
<tr>
<td>y yy</td>
<td>3.716843</td>
<td>3.716812</td>
<td>-3.2E-05</td>
</tr>
<tr>
<td>z yy</td>
<td>-0.810176</td>
<td>-0.810176</td>
<td>2.5E-05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Numerical</th>
<th>DFPT</th>
<th>Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>x yz</td>
<td>-3.871980</td>
<td>-3.872154</td>
<td>-1.7E-04</td>
</tr>
<tr>
<td>y yz</td>
<td>-1.245173</td>
<td>-1.245206</td>
<td>-3.3E-05</td>
</tr>
<tr>
<td>z yz</td>
<td>1.902687</td>
<td>1.902693</td>
<td>5.6E-06</td>
</tr>
</tbody>
</table>

- RMS Errors 4.0X10⁻⁵, ELT and 1.7X10⁻⁶, PZT
  - One-two orders of magnitude smaller errors for clamped-atom quantities.
Present status, future development

- Examples of strain RF and anaddb calculations are `Test_v4/t61-70`
- RF strain is fully parallelized
  - Parallel version was developed simultaneously with sequential
- Present limitations
  - Norm-conserving psp’s
  - Non-spin polarized (this is about to be relaxed, testing is nearly complete)
  - LDA only
  - No spin-orbit
- GGA prospects
  - Probably straightforward but complicated by “two kinds of charge” problem with model cores
  - Model core smoothness problem is undoubtedly worse
- Spin-orbit coupling
  - This has all the nonlocal psp complexity, probably significantly worse judging by the existing spin-orbit code for stress
  - *Mathematica* code will eventually be added to the documentation and may help a future developer with this
Future development, continued

• PAW
  – Far beyond norm-conserving psp non-local complexity
  – Needs spherical harmonics with off-diagonal coupling which cannot be turned into dot products with simple metric-tensor dependencies
  – Has “two kinds of charge” problem like model core but much worse, because augmentation charge has non-spherical components

On the upbeat side, however

• 3rd-order response functions involving strain via “2n+1” theorem
  – Require two $\psi^{(1)}$ and one $H^{(1)}$, all available
  – Eg., electrostriction, non-linear elastic constants, Grüneisen parameters

• It’s time for feedback – let’s see what the users want and what trouble they get into
  – If a user wants a strain feature badly enough we’ll have a new developer!
  – Isn’t that the ABINIT philosophy?
Appendix : Mathematica for nonlocal psp

\[ \langle K' | V_{NL} | K \rangle = \frac{1}{\Omega} \sum_{k'l'm} e^{iK' \cdot \tau_k} f_{k'l'}(K' \cdot K') \langle \Omega \cdot (K' \cdot K', K' \cdot K, K \cdot K) e^{-iK \cdot \tau_k} f_{k'l'}(K \cdot K). \]

- Define tensor products \( T_{\ell m} (\bar{K}) \) and \( T_{\ell m} (\bar{K}') \)
  - Follows D. C. Allan

\[
\begin{align*}
\text{tnk} &= \{ \\
&\{1\}, (* 0, 1 *) \\
&\{k1, (* 1, 1 *) \\
&k2, (* 1, 2 *) \\
&k3\}, (* 1, 3 *) \\
&\{k1 k1, (* 2, 1 *) \\
&k2 k2, (* 2, 2 *) \\
&k3 k3, (* 2, 3 *) \\
&k3 k2, (* 2, 4 *) \\
&\text{etc. to rank 7}
\end{align*}
\]

- Define \( K' \)'s, metric tensor functions, dot products, and Legendre's
- \( s1 \) and \( s2 \) are strain variables

\[
\begin{align*}
k &= \{k1, k2, k3\}; \ kp &= \{kp1, kp2, kp3\}; \\
m &= \{\{m1[1,s1,s2], m12[s1,s2], m13[s1,s2]\}, \\
&\{m12[s1,s2], m22[s1,s2], m23[s1,s2]\}, \\
&\{m13[s1,s2], m23[s1,s2], m33[s1,s2]\}\}; \\
dt &= kp.m.k; \ ks = k.m.k; \ kps = kp.m.kp; \\
Plegendre &= \{1, dt, 1.5 dt^2 - 0.5 kps ks, \\
&2.5 dt^3 - 1.5 kps dt ks\};
\end{align*}
\]
Mathematica for nonlocal psp, continued

- Strain derivatives of form factors $f_\ell$ “bring out” derivatives of dot products
- Define 6 combinations of dot product derivatives and Legendre derivatives that have given offsets between “input” and “output” rank

```
poly = {D[kps,s2] D[kps,s1] Plegendre[[rank+1]],
        D[ks, s2] D[ks, s1] Plegendre[[rank+1]],
        (D[D[kps,s2],s1] Plegendre[[rank+1]]
         + D[kps,s1] D[Plegendre[[rank+1]],s2]
         + D[kps,s2] D[Plegendre[[rank+1]],s1]),
        (D[D[ks, s2],s1] Plegendre[[rank+1]]
         + D[ks, s1] D[Plegendre[[rank+1]],s2]
         + D[ks, s2] D[Plegendre[[rank+1]],s1]),
        (D[kps,s1] D[ks,s2] + D[kps,s2] D[ks,s1])
        Plegendre[[rank+1]],
        D[D[Plegendre[[rank+1]],s2],s1]);
```

- In Mathematica $df/dx \text{ is } D[f,x]$
- Now, do the work – extract the coefficients of each pair of input and output tensors

```
Do[term = Simplify[Coefficient[poly[[iterm]],
                          (tnkp[[rankout+1]][[jj]] *
                          tnk[[rankin+1]][[ii]])]];
```
Title

- X
- X
- X
- X