

Siesta interface to AiiDA

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AiiDA workflows tutorial
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AiiDA-Siesta package

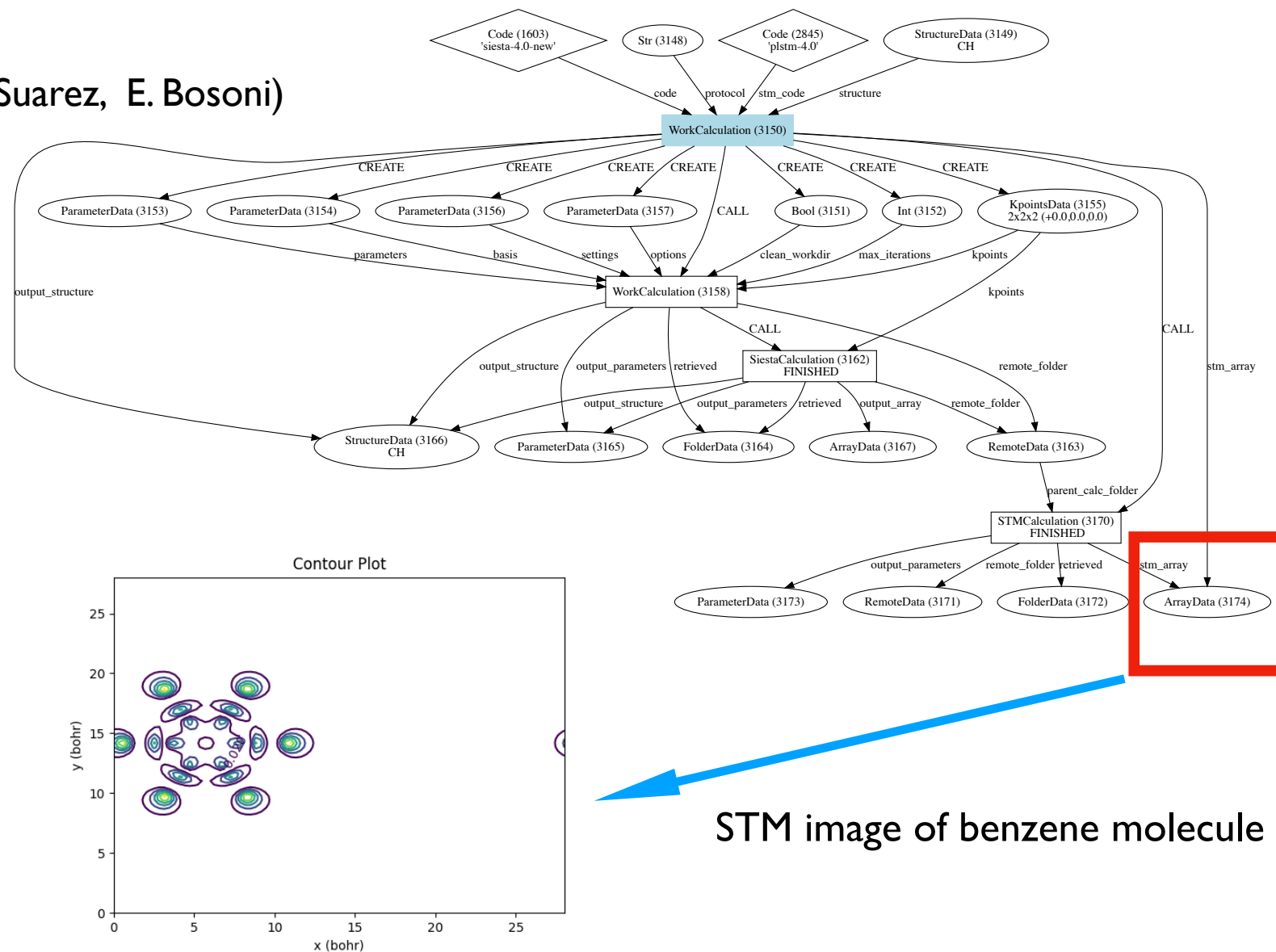
(A. Garcia, V. Dikan, V.M. Garcia-Suarez, E. Bosoni)

Plugin

- Total energies, forces, stresses, bands, spin polarization.
- Geometry relaxations (including variable cell), but no MD yet (no trajectories in the plugin).
- Output plugin uses existing CML I/O framework in XML.
- Basic mechanism for error reporting and restarts has been implemented.
- Incorporates new “Psfddata” class for pseudopotentials.
- All of Siesta FDF constructs can be passed to the plugin in the ‘parameters’ dictionary. So most of Siesta is in principle covered, except that the parsing is limited.

Workflows

- **BaseWorkChain:** Supports the basic features of SIESTA. It can recover from lack of convergence or out-of-time conditions.
- **BandsWorkChain:** Harnesses the Base workflow to compute the band structure.
- **STMWorkChain:** Computes the LDOS as a proxy for STM images,



```
"entry_points": {  
    "aiida.calculations": [  
        "siesta.siesta = aiida_siesta.calculations.siesta:SiestaCalculation",  
        "siesta.stm = aiida_siesta.calculations.stm:STMCalculation",  
        "siesta.vibra = aiida_siesta.calculations.vibra:VibraCalculation"  
    ],  
    "aiida.parsers": [  
        "siesta.parser = aiida_siesta.parsers.siesta:SiestaParser",  
        "siesta.stm = aiida_siesta.parsers.stm:STMParser",  
        "siesta.vibra = aiida_siesta.parsers.vibra:VibraParser"  
    ],  
    "aiida.data": [  
        "siesta.psf = aiida_siesta.data.psf:PsfData"  
    ],  
    "aiida.cmdline.data": [  
        "psf = aiida_siesta.commands.data_psf:psfdata"  
    ]  
}
```

Inputs

code:	required	Code	Input code
parameters:	required	Dict	Input parameters
pseudos:	required	PsfData	Input pseudo potentials
structure:	required	StructureData	Input structure
bandskpoints:	optional	KpointsData	Input kpoints for bands
basis:	optional	Dict	Input basis
kpoints:	optional	KpointsData	Input kpoints
metadata:	optional		
parent_calc_folder:	optional	RemoteData	Parent folder
settings:	optional	Dict	Input settings

Outputs

output_parameters:	required	Dict	The calculation results
remote_folder:	required	RemoteData	Input files necessary to run the process will be retrieved from this folder node ...
retrieved:	required	FolderData	Files that are retrieved by the daemon will be stored in this folder node ...
bands_array:	optional	BandsData	Optional band structure
bands_parameters:	optional	Dict	Optional parameters of bands
forces_and_stress:	optional	ArrayData	Optional forces and stress
output_structure:	optional	StructureData	Optional relaxed structure

Exit codes

10:	The process returned an invalid output
11:	The process did not register a required output
100:	The retrieved folder data node could not be accessed.
120:	Calculation did not reach scf convergence!
130:	Calculation did not reach geometry convergence!

```

alat = 15. # angstrom
cell = [[alat, 0., 0.],
        [0., alat, 0.],
        [0., 0., alat],
        ]

# Benzene molecule with a special carbon atom
s = StructureData(cell=cell)
s.append_atom(position=(0.000,0.000,0.468),symbols=['H'])
s.append_atom(position=(0.000,0.000,1.620),symbols=['C'])
s.append_atom(position=(0.000,-2.233,1.754),symbols=['H'])
s.append_atom(position=(0.000,2.233,1.754),symbols=['H'])
s.append_atom(position=(0.000,-1.225,2.327),symbols='C',name="Cred")
s.append_atom(position=(0.000,1.225,2.327),symbols=['C'])
s.append_atom(position=(0.000,-1.225,3.737),symbols=['C'])
s.append_atom(position=(0.000,1.225,3.737),symbols=['C'])
s.append_atom(position=(0.000,-2.233,4.311),symbols=['H'])
s.append_atom(position=(0.000,2.233,4.311),symbols=['H'])
s.append_atom(position=(0.000,0.000,4.442),symbols=['C'])
s.append_atom(position=(0.000,0.000,5.604),symbols=['H'])

```

```

pseudo_file_to_species_map = [ ("C.psf", ['C', 'Cred']),
                                ("H.psf", 'H')
                              ]

```

```

basis_dict = {
'pao-basistype': 'split',
'pao-splitnorm': 0.150,
'pao-energyshift': '0.020 Ry',
'%block pao-basis-sizes' :""
C      SZP
Cred SZ
H      SZP
%endblock pao-basis-sizes"",
}

```

Output

```

{
  "siesta:Version": "siesta-4.0.2",
  "E_fermi": -3.24,
  "E_fermi_units": "eV",
  "FreeE": -6656.2343
  "FreeE_units": "eV",
  "global_time": 55.213,
  "timing_decomposition": {
    "compute_DM": 33.208,
    "nlefsm-1": 0.582,
    "nlefsm-2": 0.045,
    "post-SCF": 2.556,
    "setup_H": 16.531,
    "setup_H0": 2.351,
    "siesta": 55.213,
    "state_init": 0.171
  },
  "warnings": [ "INFO: Job Completed" ]
}

```

Pre-packaged quality protocols

Work-in-Progress
Example from QE:

```
self.ctx.protocol = {  
    'kpoints_mesh_offset': [0., 0., 0.],  
    'kpoints_mesh_density': 0.2,  
    'convergence_threshold': 2.E-06,  
    'smearing': 'marzari-vanderbilt',  
    'degauss': 0.02,  
    'occupations': 'smearing',  
    'tstress': True,  
    'pseudo_data': {  
        'H': {'cutoff': 55, 'dual': 8, 'pseudo': '031US'},  
        'He': {'cutoff': 55, 'dual': 4, 'pseudo': 'SG15'},  
        'Li': {'cutoff': 30, 'dual': 8, 'pseudo': 'GBRV-1.4'},  
        'Be': {'cutoff': 40, 'dual': 8, 'pseudo': 'GBRV-1.4'},  
        'B': {'cutoff': 40, 'dual': 8, 'pseudo': '031PAW'},
```

We need to provide a more comprehensive
pseudopotential database

PSML format available

Help me

PSEUDŌ DŌJŌ

Download

Type NC (ONCVSP v0.4) **XC** PBE **Accuracy** standard

3.13 Mean

psp8
upf
psml
✓ html
djrepo

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Select the flavor and [format](#), then click "Download" to get the complete table of pseudos or choose a specific element. "HTML" gives full test results.

1 H 1 32 0.1 38 2.5 42 -0.00 Hydrogen	2 He 1 39 0.0 45 4.2 49 na Helium
3 Li 2 33 0.2 37 1.9 41 -0.10 Lithium	4 Be 2 38 1.4 44 4.4 50 0.20 Beryllium
11 Na 3 38 0.4 44 4.6 48 -0.00 Sodium	12 Mg 3 38 0.4 42 1.5 48 0.00 Magnesium
19 K 3 33 0.2 37 2.0 43 -0.30 Potassium	20 Ca 3 28 0.1 34 0.3 38 -0.20 Calcium
21 Sc 4 35 1.3 39 2.8 45 -0.00 Scandium	22 Ti 4 38 0.9 42 1.3 46 -0.00 Titanium
23 V 4 38 1.3 42 1.6 48 -0.10 Vanadium	24 Cr 4 43 10.5 47 18.1 55 -0.00 Chromium
25 Mn 4 42 8.0 48 16.9 54 -0.10 Manganese	26 Fe 4 41 5.6 45 9.2 53 -0.10 Iron
27 Co 4 42 1.0 48 1.4 54 -0.00 Cobalt	28 Ni 4 45 1.5 49 1.5 55 -0.10 Nickel
29 Cu 4 48 0.9 52 -0.10 Copper	30 Zn 4 48 0.8 52 -0.10 Zinc
31 Ga 3 36 0.5 40 1.5 46 -0.00 Gallium	32 Ge 3 35 0.5 39 1.0 45 -0.00 Germanium
33 As 3 38 0.4 42 0.7 48 -0.00 Arsenic	34 Se 3 39 0.2 43 0.5 49 -0.10 Selenium
35 Br 2 19 0.0 23 0.2 29 -0.20 Bromine	36 Kr 2 22 0.0 26 2.3 34 na Krypton
37 Rb 3 19 0.2 23 2.9 29 -0.40 Rubidium	38 Sr 3 28 1.3 34 6.1 40 -0.20 Strontium
39 Y 4 30 1.0 36 2.3 42 -0.10 Yttrium	40 Zr 4 29 0.8 33 1.1 49 -0.00 Zirconium
41 Nb 4 37 1.3 41 1.3 49 -0.00 Niobium	42 Mo 4 36 1.4 40 1.0 46 -0.10 Molybdenum
43 Tc 4 38 1.6 42 1.1 48 -0.00 Technetium	44 Ru 4 38 2.1 42 1.5 50 -0.00 Ruthenium
45 Rh 4 40 2.6 44 2.1 50 -0.00 Rhodium	46 Pd 3 37 1.1 41 1.3 49 -0.10 Palladium
47 Ag 4 37 0.3 41 0.6 47 -0.10 Silver	48 Cd 4 47 1.1 51 3.5 57 -0.00 Cadmium
49 In 3 31 0.1 35 0.2 41 -0.10 Indium	50 Sn 3 32 0.8 36 1.8 42 0.00 Tin
51 Sb 3 36 0.5 40 1.0 44 0.00 Antimony	52 Te 3 34 0.8 40 1.6 46 0.10 Tellurium
53 I 2 31 0.4 35 1.1 41 0.00 Iodine	54 Xe 2 28 0.0 34 2.5 42 na Xenon
55 Cs 3 19 0.1 25 1.5 29 -0.40 Caesium	56 Ba 3 18 0.9 22 4.9 28 -0.10 Barium
72 Hf 4 25 0.6 29 0.8 35 -0.00 Hafnium	73 Ta 4 25 0.7 29 0.6 35 -0.10 Tantalum
74 W 4 31 0.2 37 0.1 41 -0.00 Wolfram	75 Re 4 30 0.7 36 0.4 42 -0.10 Rhenium
76 Os 4 33 1.7 37 0.9 43 -0.10 Osmium	77 Ir 4 34 1.5 38 0.9 44 -0.20 Iridium
78 Pt 4 38 0.6 42 0.5 50 -0.20 Platinum	79 Au 4 32 1.3 38 1.6 44 -0.10 Gold
80 Hg 4 29 0.7 33 7.2 39 na Mercury	81 Tl 3 27 0.1 31 0.2 37 -0.10 Thallium
82 Pb 3 24 0.1 28 0.1 34 -0.10 Lead	83 Bi 3 29 0.2 33 0.4 37 -0.00 Bismuth
84 Po 3 28 0.3 32 0.5 38 na Polonium	85 At 3 na na na na Astatine
86 Rn 3 32 0.0 36 2.4 42 na Radon	
104 Rf 4 25 0.6 29 0.8 35 -0.00 Rutherfordium	105 Db 4 25 0.7 29 0.6 35 -0.10 Dubnium
106 Sg 4 31 0.2 37 0.1 41 -0.00 Seaborgium	107 Bh 4 30 0.7 36 0.4 42 -0.10 Bohrium
108 Hs 4 33 1.7 37 0.9 43 -0.10 Hassium	109 Mt 4 34 1.5 38 0.9 44 -0.20 Meitnerium
110 Ds 4 38 0.6 42 0.5 50 -0.20 Darmstadtium	111 Rg 4 32 1.3 38 1.6 44 -0.10 Roentgenium
112 Cn 4 29 0.7 33 7.2 39 na Copernicium	113 Nh 3 27 0.1 31 0.2 37 -0.10 Nihonium
114 Fl 3 24 0.1 28 0.1 34 -0.10 Flerovium	115 Mc 3 29 0.2 33 0.4 37 -0.00 Moscovium
116 Lv 3 28 0.3 32 0.5 38 na Livermorium	117 Ts 3 28 0.5 32 0.5 38 na Tennessine
118 Og 3 32 0.0 36 2.4 42 na Oganesson	
57 La 4 50 na 55 -0.10 Lanthanum	58 Ce na na na na na Cerium
59 Pr na na na na na Praseodymium	60 Nd na na na na na Neodymium
61 Pm na na na na na Promethium	62 Sm na na na na na Samarium
63 Eu na na na na na Europium	64 Gd na na na na na Gadolinium
65 Tb na na na na na Terbium	66 Dy na na na na na Dysprosium
67 Ho na na na na na Holmium	68 Er na na na na na Erbium
69 Tm na na na na na Thulium	70 Yb na na na na na Ytterbium
71 Lu 5 46 1.0 50 2.2 58 na Lutetium	
89 Ac 4 25 0.6 29 0.8 35 -0.00 Actinium	90 Th 4 25 0.7 29 0.6 35 -0.10 Thorium
91 Pa 4 25 0.7 29 0.6 35 -0.10 Protactinium	92 U 4 25 0.7 29 0.6 35 -0.10 Uranium
93 Np 4 25 0.7 29 0.6 35 -0.10 Neptunium	94 Pu 4 25 0.7 29 0.6 35 -0.10 Plutonium
95 Am 4 25 0.7 29 0.6 35 -0.10 Americium	96 Cm 4 25 0.7 29 0.6 35 -0.10 Curium
97 Bk 4 25 0.7 29 0.6 35 -0.10 Berkelium	98 Cf 4 25 0.7 29 0.6 35 -0.10 Californium
99 Es 4 25 0.7 29 0.6 35 -0.10 Einsteinium	100 Fm 4 25 0.7 29 0.6 35 -0.10 Fermium
101 Md 4 25 0.7 29 0.6 35 -0.10 Mendelevium	102 No 4 25 0.7 29 0.6 35 -0.10 Nobelium
103 Lr 4 25 0.7 29 0.6 35 -0.10 Lawrencium	

Other Issues

- **Basis sets** are further away from being treated as a “black-box”. We have some high-level knobs in Siesta, but some more heuristics are needed.
- **More features** need to be implemented and tested in the plugins and the workflows.
- **Migration** to 1.0 almost completed.
- A proper **taxonomy of failure modes** is needed

<http://aiida-siesta-plugin.readthedocs.io>

From Siesta to AiiDA and back

- While designing the plugin and workflows, **new ideas** for SIESTA operation appeared:
 - Proper **error reporting**
 - Production of more files, easier to **parse**.
 - Re-modularization; new basic objects
- New **insights**:
 - Codes are already implementing **crude workflows**
 - Separation of functionality is a key issue

Thank you