XML support in the QE-GIPAW code

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1 Introduction

Since version 7.0, QE-GIPAW[1] creates an XML file at the end of a calculation which includes: general information about the run job, parallelization and timing info, input parameters and relevant results (NMR shielding tensors, electric field gradients, EPR Δg, hyperfine coupling parameters). This set of physical quantities will be extended to include J-couplings, Mössbauer parameter and ZFS.

The XML facility is implemented in `src/gipaw_results.f90` and `src/xml_routines.f90`. The first source file is a place-holder for the NMR and EPR parameters to be written to the XML file. The second source file implements the actual writing of the XML file, using directly the FoX library and pre-procesor tricks. This choice is because the number of variables to be dumped (both inout and output) is limited and the format of XML file is not expected to be changed frequently, in a post-processing code like QE-GIPAW.

2 GIPAW schema

The GIPAW schema imports from the QES schema (2021-11-10). It is found in the `schema` directory and it is reported in the appendix. The root element is `gpw:gipaw`. We used `all` instead of `sequence` to allow XML tags in any order. This can be changed easily, if needed.

QE-GIPAW does not overwrite or append to the PW XML file. QE-GIPAW creates *prefix*`-gipaw.xml` in the `outdir` directory. This way the validity of both PW and GIPAW XML files can be checked with the following script:

```
# validate PW XML file
$ xmllint --noout --schema qes_211101.xsd PREFIX.xml

# validate GIPAW XML file
$ xmllint --noout --schema gipaw_xmlschema_import_local.xsd PREFIX-gipaw.xml
```

3 Utilities

In the directory `schema/` we provide the following utilities:

- `validate.sh`: validates both the PW and GIPAW XML files against the schemas
- `gipawxml_dump.py`: dumps in human-readable format the NMR/EPR parameters from the XML file. It can be used as a starting point for GUI integration.
- `gipawxml_to_namelist.py`: converts the GIPAW XML file back to the GIPAW input Fortran namelist

[1] `https://github.com/dceresoli/qe-gipaw`

A Appendix

A.1 GIPAW XML schema

```
<?xml version="1.0"?>
<schema xmlns="http://www.w3.org/2001/XMLSchema"
        xmlns:qes="http://www.quantum-espresso.org/ns/qes/qes-1.0"
        xmlns:gpw="http://www.quantum-espresso.org/ns/gpw/qes_gipaw_1.0"
        targetNamespace="http://www.quantum-espresso.org/ns/gpw/qes_gipaw_1.0">
        <import schemaLocation="http://www.quantum-espresso.org/ns/qes/qes_211101.xsd" namespace="http://
             www.quantum-espresso.org/ns/qes/qes-1.0"/>

    <!-- QE-GIPAW (root element) -->
    <element name="gipaw" type="gpw:gipawType" />

    <complexType name="gipawType">
        <all>
            <element type="qes:general_infoType" name="general_info" minOccurs="0"/>
            <element type="qes:parallel_infoType" name="parallel_info" minOccurs="0"/>
            <element type="gpw:inputGIPAWType" name="input" />
            <element type="gpw:outputGIPAWType" name="output" minOccurs="0" />
            <element type="qes:statusType" name="exit_status" minOccurs="0" />
            <element type="qes:closedType" name="closed" minOccurs="0" />
            <element type="qes:timingType" name="timing_info" minOccurs="0" />
        </all>
    </complexType>


    <!-- vector types -->
    <!-- bool array da spostare in qes  -->
    <simpleType name="boolvectorType">
        <restriction>
            <simpleType>
                <list itemType="boolean"/>
            </simpleType>
        </restriction>
    </simpleType>

    <complexType name="atomTensorList">
        <sequence>
            <element type="gpw:atomtensor" name="atom" maxOccurs="unbounded" />
        </sequence>
     </complexType>

     <complexType name="atomtensor">
         <simpleContent>
             <extension base="qes:matrixType">
                 <attribute type="string" name="name" />
                 <attribute type="string" name="tau" />
                 <attribute type="string" name="units" />
                 <attribute type="positiveInteger" name="index" />
             </extension>
         </simpleContent>
     </complexType>


    <!-- enumerations -->
    <simpleType name="JobType">
        <restriction base="string">
            <enumeration value="nmr"/>
            <enumeration value="efg"/>
            <enumeration value="g_tensor"/>
            <enumeration value="hyperfine"/>
            <enumeration value="mossbauer"/>
        </restriction>
    </simpleType>

    <simpleType name="RestartModeType">
        <restriction base="string">
            <enumeration value="from_scratch"/>
            <enumeration value="restart"/>
        </restriction>
    </simpleType>

    <simpleType name="VerbosityType">
        <restriction base="string">
```

```
        <enumeration value="low"/>
        <enumeration value="medium"/>
        <enumeration value="high"/>
    </restriction>
</simpleType>

<simpleType name="DiagonalizationType">
    <restriction base="string">
        <enumeration value="cg"/>
        <enumeration value="david"/>
    </restriction>
</simpleType>

<simpleType name="HFIOutputUnitType">
    <restriction base="string">
        <enumeration value="MHz"/>
        <enumeration value="mT"/>
        <enumeration value="G"/>
        <enumeration value="10e-4cm^-1"/>
    </restriction>
</simpleType>


<!-- INPUTGIPAW TYPE-->
<complexType name="inputGIPAWType">
    <all>
        <element type="gpw:JobType" name="job" default="nmr" minOccurs="0" />
        <element type="gpw:RestartModeType" name="restart_mode" default="from_scratch" minOccurs="0"
            />
        <element type="gpw:VerbosityType" name="verbosity" default="low" minOccurs="0" />
        <element type="double" name="max_seconds" default="1e7" minOccurs="0" />

        <element type="string" name="prefix" default="pwscf" minOccurs="0" />
        <element type="string" name="tmp_dir" default="./" minOccurs="0" />
        <element type="string" name="filcurr" default="" minOccurs="0" />
        <element type="string" name="filfield" default="" minOccurs="0" />
        <element type="string" name="filnics" default="" minOccurs="0" />

        <element type="gpw:DiagonalizationType" name="diagonalization" default="david" minOccurs="0"
            />
        <element type="double" name="conv_threshold" default="1e-14" minOccurs="0" />
        <element type="double" name="q_gipaw" default="0.01" minOccurs="0" />
        <element type="double" name="r_rand" default="0.1" minOccurs="0" />
        <element type="boolean" name="spline_ps" default="true" minOccurs="0" />
        <element type="gpw:boolvectorType" name="pawproj" default="false" minOccurs="0" />

        <element type="boolean" name="use_nmr_macroscopic_shape" default="true" minOccurs="0" />
        <element type="qes:matrixType" name="nmr_macroscopic_shape"
                 default="0.666667␣0.000000␣0.000000␣0.000000␣0.666667␣0.000000␣0.000000␣0.000000␣
                     0.666667" minOccurs="0" />

        <element type="qes:vectorType" name="q_efg" default="0.0" minOccurs="0" />

        <element type="gpw:HFIOutputUnitType" name="hfi_output_unit" default="MHz" minOccurs="0" />
        <element type="qes:vectorType" name="hfi_nuclear_g_factor" default="0.0" minOccurs="0" />
        <element type="integer" name="core_relax_method" default="0" minOccurs="0" />
        <element type="boolean" name="hfi_via_reconstruction_only" default="false" minOccurs="0" />

    </all>
</complexType>


<!-- OUTPUTGIPAW TYPE -->
<complexType name="outputGIPAWType">
    <all>
        <element type="qes:matrixType" name="susceptibility_low" minOccurs="0" />
        <element type="qes:matrixType" name="susceptibility_high" minOccurs="0" />

        <element type="gpw:atomTensorList" name="shielding_tensors" minOccurs="0" />

        <element type="qes:matrixType" name="delta_g" minOccurs="0" />
        <element type="qes:matrixType" name="delta_g_paratec" minOccurs="0" />

        <element type="gpw:atomTensorList" name="electric_field_gradients" minOccurs="0" />

        <element type="gpw:atomTensorList" name="hyperfine_dipolar" minOccurs="0" />
        <element type="gpw:atomTensorList" name="hyperfine_fermi_contact" minOccurs="0" />
```

```
        </all>
      </complexType>


</schema>
```

A.2 Example GIPAW XML file: benzene-gipaw.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<gpw:gipaw xsi:schemaLocation="http://www.quantum-espresso.org/ns/gpw/qes_gipaw_1.0␣http://www.quantum-
    espresso.org/ns/gpw/gpw_202201.xsd" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:qes=
    "http://www.quantum-espresso.org/ns/qes/qes-1.0" xmlns:gpw="http://www.quantum-espresso.org/ns/gpw/
    qes_gipaw_1.0">
  <general_info>
    <xml_format NAME="QEXSD" VERSION="21.07.16">QEXSD_21.07.16</xml_format>
    <creator NAME="GIPAW" VERSION="5d0ab5847c1e35afc9e496ae7002918c7228aed9">XML file generated by GIPAW<
        /creator>
    <created DATE="13Jan2022" TIME="13:27:16␣">This run was terminated on:  13:27:16  13 Jan 2022</
        created>
    <job/>
  </general_info>
  <parallel_info>
    <nprocs>4</nprocs>
    <nthreads>1</nthreads>
    <ntasks>1</ntasks>
    <nbgrp>1</nbgrp>
    <npool>1</npool>
    <ndiag>4</ndiag>
  </parallel_info>
  <input>
    <job>nmr</job>
    <prefix>benzene</prefix>
    <tmp_dir>./scratch/</tmp_dir>
    <conv_threshold>1.000000000000e-14</conv_threshold>
    <restart_mode>restart</restart_mode>
    <q_gipaw>1.000000000000e-2</q_gipaw>
    <verbosity>high</verbosity>
    <filcurr></filcurr>
    <filfield></filfield>
    <filnics></filnics>
    <pawproj>false false false false false false false false false false</pawproj>
    <use_nmr_macroscopic_shape>false</use_nmr_macroscopic_shape>
    <nmr_macroscopic_shape rank="2" dims="3␣3">6.666666666667e-1 0.000000000000e0 0.000000000000e0
        0.000000000000e0 6.666666666667e-1 0.000000000000e0 0.000000000000e0 0.000000000000e0
        6.666666666667e-1</nmr_macroscopic_shape>
    <spline_ps>true</spline_ps>
    <diagonalization>cg</diagonalization>
    <q_efg size="12">1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0
         1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0</q_efg>
    <max_seconds>1.000000000000e7</max_seconds>
    <r_rand>1.000000014901e-1</r_rand>
    <hfi_output_unit>MHz</hfi_output_unit>
    <hfi_nuclear_g_factor size="12">1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0
        1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0 1.000000000000e0
        1.000000000000e0</hfi_nuclear_g_factor>
    <core_relax_method>1</core_relax_method>
    <hfi_via_reconstruction_only>false</hfi_via_reconstruction_only>
  </input>
  <output>
    <susceptibility_low rank="2" dims="3␣3">-3.766897012885e1 0.000000000000e0 0.000000000000e0
        0.000000000000e0 -3.758749014540e1 0.000000000000e0 0.000000000000e0 0.000000000000e0
        -8.742266962391e1</susceptibility_low>
    <susceptibility_high rank="2" dims="3␣3">-3.288895459326e1 0.000000000000e0 0.000000000000e0
        0.000000000000e0 -3.279761874576e1 0.000000000000e0 0.000000000000e0 0.000000000000e0
        -9.361335676347e1</susceptibility_high>
    <shielding_tensors>
      <atom name="C" tau="0.000000000000e0␣1.076792509380e-1␣0.000000000000e0" index="1" rank="2" dims="3
          ␣3" units="ppm">3.167358934721e1 -9.740878520583e-15 -2.067575271274e-16 3.557538406442e-14
          -6.703902201518e1 6.182700274579e-17 -6.795402634274e-17 4.685255109366e-16 1.687121260440e2</
          atom>
      <atom name="C" tau="9.325297833381e-2␣5.383962546900e-2␣0.000000000000e0" index="2" rank="2" dims="
          3␣3" units="ppm">-4.244860653598e1 -4.275946419992e1 1.907346085370e-16 -4.276559411826e1
          6.955670087686e0 8.444949960056e-17 5.868135969236e-16 4.056616206048e-16 1.687711176044e2</
          atom>
      <atom name="C" tau="9.325297833381e-2␣-5.383962546900e-2␣0.000000000000e0" index="3" rank="2" dims=
```

```
      "3␣3" units="ppm">-4.244860653598e1 4.275946419992e1 1.492868154958e-16 4.276559411826e1
      6.955670087686e0 5.555332652616e-17 7.081128084320e-16 -1.397920184527e-16 1.687711176044e2</
      atom>
  <atom name="C" tau="0.000000000000e0␣-1.076792509380e-1␣0.000000000000e0" index="4" rank="2" dims="
      3␣3" units="ppm">3.167358934721e1 -4.658681209067e-15 5.897216238067e-17 4.086933970585e-14
      -6.703902201518e1 4.424524861514e-17 7.088675311687e-17 -2.409577394549e-16 1.687121260440e2</
      atom>
  <atom name="C" tau="-9.325297833381e-2␣-5.383962546900e-2␣0.000000000000e0" index="5" rank="2" dims
      ="3␣3" units="ppm">-4.244860653598e1 -4.275946419992e1 3.686773737353e-17 -4.276559411826e1
      6.955670087686e0 1.348985234123e-16 -8.123074693337e-16 2.796255306431e-16 1.687711176044e2</
      atom>
  <atom name="C" tau="-9.325297833381e-2␣5.383962546900e-2␣0.000000000000e0" index="6" rank="2" dims=
      "3␣3" units="ppm">-4.244860653598e1 4.275946419992e1 -3.345021225355e-16 4.276559411826e1
      6.955670087686e0 2.280119461582e-16 -4.177679511712e-16 3.319758668613e-16 1.687711176044e2</
      atom>
  <atom name="H" tau="0.000000000000e0␣1.915227445285e-1␣0.000000000000e0" index="7" rank="2" dims="3
      ␣3" units="ppm">2.358056445746e1 -1.609362599783e-14 -1.973055769479e-16 -3.917527381051e-15
      2.337861659521e1 4.792078293236e-17 2.549891058796e-17 7.667413752936e-16 2.056760805236e1</
      atom>
  <atom name="H" tau="1.658635305849e-1␣9.576133358251e-2␣0.000000000000e0" index="8" rank="2" dims="
      3␣3" units="ppm">2.339493036332e1 -1.844984037033e-1 1.388154335765e-16 -1.843204720044e-1
      2.357165617950e1 2.207332836292e-16 6.209133536853e-16 4.213850284511e-16 2.057308237006e1</
      atom>
  <atom name="H" tau="1.658635305849e-1␣-9.576133358251e-2␣0.000000000000e0" index="9" rank="2" dims=
      "3␣3" units="ppm">2.339493036332e1 1.844984037032e-1 4.983314750962e-17 1.843204720043e-1
      2.357165617950e1 -5.299473472390e-17 6.880748022507e-16 -1.482378937892e-16 2.057308237006e1</
      atom>
  <atom name="H" tau="0.000000000000e0␣-1.915227445285e-1␣0.000000000000e0" index="10" rank="2" dims=
      "3␣3" units="ppm">2.358056445746e1 -1.567010952420e-14 -4.668218424160e-18 -2.117582368136e-16
       2.337861659521e1 -8.424693425998e-17 -2.338112078921e-16 -4.762745264707e-16 2.056760805236e1
      </atom>
  <atom name="H" tau="-1.658635305849e-1␣-9.576133358251e-2␣0.000000000000e0" index="11" rank="2"
      dims="3␣3" units="ppm">2.339493036332e1 -1.844984037033e-1 -1.049251978430e-17 -1.843204720044
      e-1 2.357165617950e1 -1.370321659825e-16 -9.134018249208e-16 -1.325386288650e-16
      2.057308237006e1</atom>
  <atom name="H" tau="-1.658635305849e-1␣9.576133358251e-2␣0.000000000000e0" index="12" rank="2" dims
      ="3␣3" units="ppm">2.339493036332e1 1.844984037032e-1 -1.355540548966e-16 1.843204720043e-1
      2.357165617950e1 -9.936415874296e-17 -7.033972893140e-16 3.368005581077e-16 2.057308237006e1</
      atom>
</shielding_tensors>
<delta_g rank="2" dims="3␣3">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
    0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</delta_g>
<delta_g_paratec rank="2" dims="3␣3">0.000000000000e0 0.000000000000e0 0.000000000000e0
    0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
    0.000000000000e0</delta_g_paratec>
<electric_field_gradients>
  <atom name="C" tau="0.000000000000e0␣1.076792509380e-1␣0.000000000000e0" index="1" rank="2" dims="3
      ␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="C" tau="9.325297833381e-2␣5.383962546900e-2␣0.000000000000e0" index="2" rank="2" dims="
      3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="C" tau="9.325297833381e-2␣-5.383962546900e-2␣0.000000000000e0" index="3" rank="2" dims=
      "3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="C" tau="0.000000000000e0␣-1.076792509380e-1␣0.000000000000e0" index="4" rank="2" dims="
      3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="C" tau="-9.325297833381e-2␣-5.383962546900e-2␣0.000000000000e0" index="5" rank="2" dims
      ="3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="C" tau="-9.325297833381e-2␣5.383962546900e-2␣0.000000000000e0" index="6" rank="2" dims=
      "3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="H" tau="0.000000000000e0␣1.915227445285e-1␣0.000000000000e0" index="7" rank="2" dims="3
      ␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="H" tau="1.658635305849e-1␣9.576133358251e-2␣0.000000000000e0" index="8" rank="2" dims="
      3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="H" tau="1.658635305849e-1␣-9.576133358251e-2␣0.000000000000e0" index="9" rank="2" dims=
      "3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="H" tau="0.000000000000e0␣-1.915227445285e-1␣0.000000000000e0" index="10" rank="2" dims=
      "3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
      0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  <atom name="H" tau="-1.658635305849e-1␣-9.576133358251e-2␣0.000000000000e0" index="11" rank="2"
```

```
        dims="3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
        0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
    <atom name="H" tau="-1.658635305849e-1␣9.576133358251e-2␣0.000000000000e0" index="12" rank="2" dims
        ="3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
        0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
  </electric_field_gradients>
  <hyperfine_dipolar>
    <atom name="C" tau="0.000000000000e0␣1.076792509380e-1␣0.000000000000e0" index="1" rank="2" dims="3
        ␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
        0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
    <atom name="C" tau="9.325297833381e-2␣5.383962546900e-2␣0.000000000000e0" index="2" rank="2" dims="
        3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
        0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0</atom>
    <atom name="C" tau="9.325297833381e-2␣-5.383962546900e-2␣0.000000000000e0" index="3" rank="2" dims=
        "3␣3" units="MHz">0.000000000000e0 0.000000000000e0 0.000000000000e0 0.000000000000e0
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